Supporting Information

Lehualides E-K, Cytotoxic Metabolites from the Tongan Marine Sponge *Plakortis* sp.

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Lehualide E (**5**)

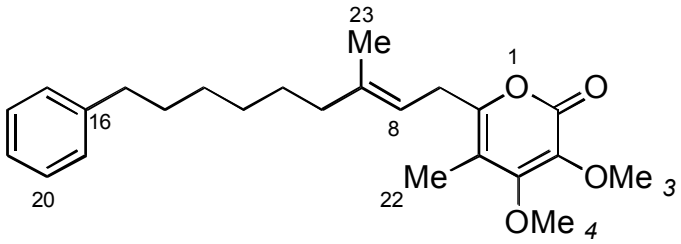


Table S 1. NMR Spectroscopic Data ($CDCl_3$, ^1H 600 MHz; ^{13}C 150 MHz) of Lehualide E (**5**).

		5			
position	**δ_C , mult**	**δ_H (*J*, Hz)**	**COSY**	**HMBC (H → C)**	**NOE[a]**
2	162.7, C				
3	128.3, C				
OCH_3 3	60.5, CH_3	3.81, s		3	*O*CH_3 4
4	159.0, C				
OCH_3 4	60.6, CH_3	4.19, s		4	*O*CH_3 3; 22
5	108.3, C				
6	154.8, C				
7	30.3, CH_2	3.17, d (6.9)	7; 22*	8; 6; 23; 5[b]	23
8	117.5, CH	5.17, t (7.2)	6; 23	7; 23; 6[b]	10
9	138.7, C				
10	39.7, CH_2	1.96, t (7.5)	10; 23	11; 23; 9; 8	8
11	27.8, CH_2		11; 9	10; 12; 9	23
12	29.9, CH_2				
13	29.3, CH_2	1.33, quin (7.3)	13; 11		
14	31.6, CH_2	1.59, quin (8.1)	14; 12	15; 16; 13	
15	36.1, CH_2	2.57, t (7.7)	13	14; 16; 17; 21	
16	143.0, C				
17	128.5, CH	7.19, d (7.4)	18	19; 21	
18	128.4, CH	7.29, t (7.0)	17; 19	16; 20	
19	125.7, CH	7.19, t (7.8)	18; 20	17; 21	
20	128.4, CH	7.29, t (7.0)	19; 21	16; 18	
21	128.5, CH	7.19, d (7.4)	20	17; 19	
22	10.3, CH_3	1.85, s	7*	5; 4; 6; 7[b]	*O*CH_3 3; 7
23	16.4, CH_3	1.66, s		9; 8; 10	11; 7

[a] Selected correlations

[b] Weak correlation

Figure S 1. 1H NMR spectrum (CDCl3, 1H 600 MHz) of lehualide E (5).

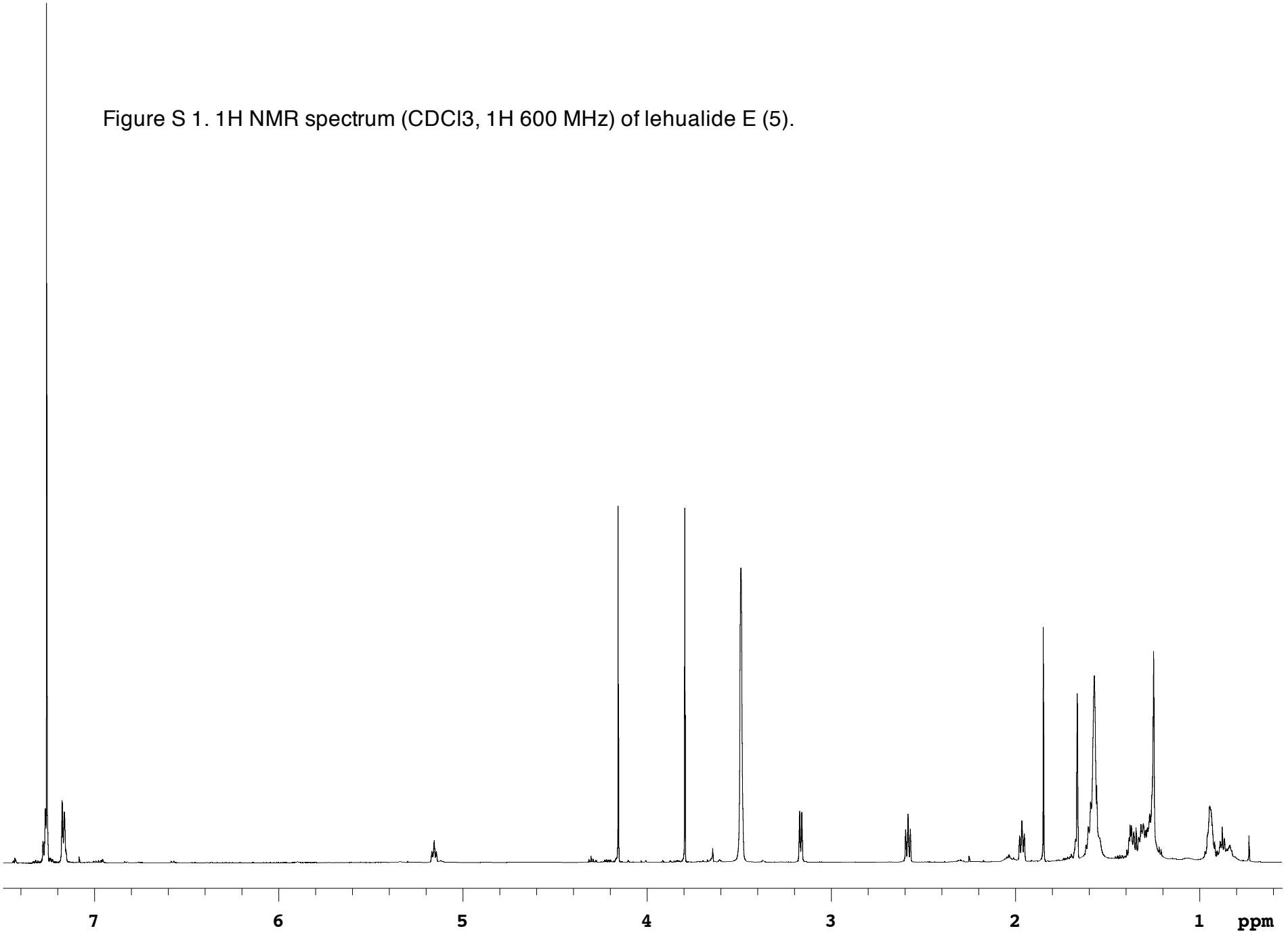


Figure S 2. COSY spectrum (CDCl3, 1H 600 MHz) of lehualide E (5).

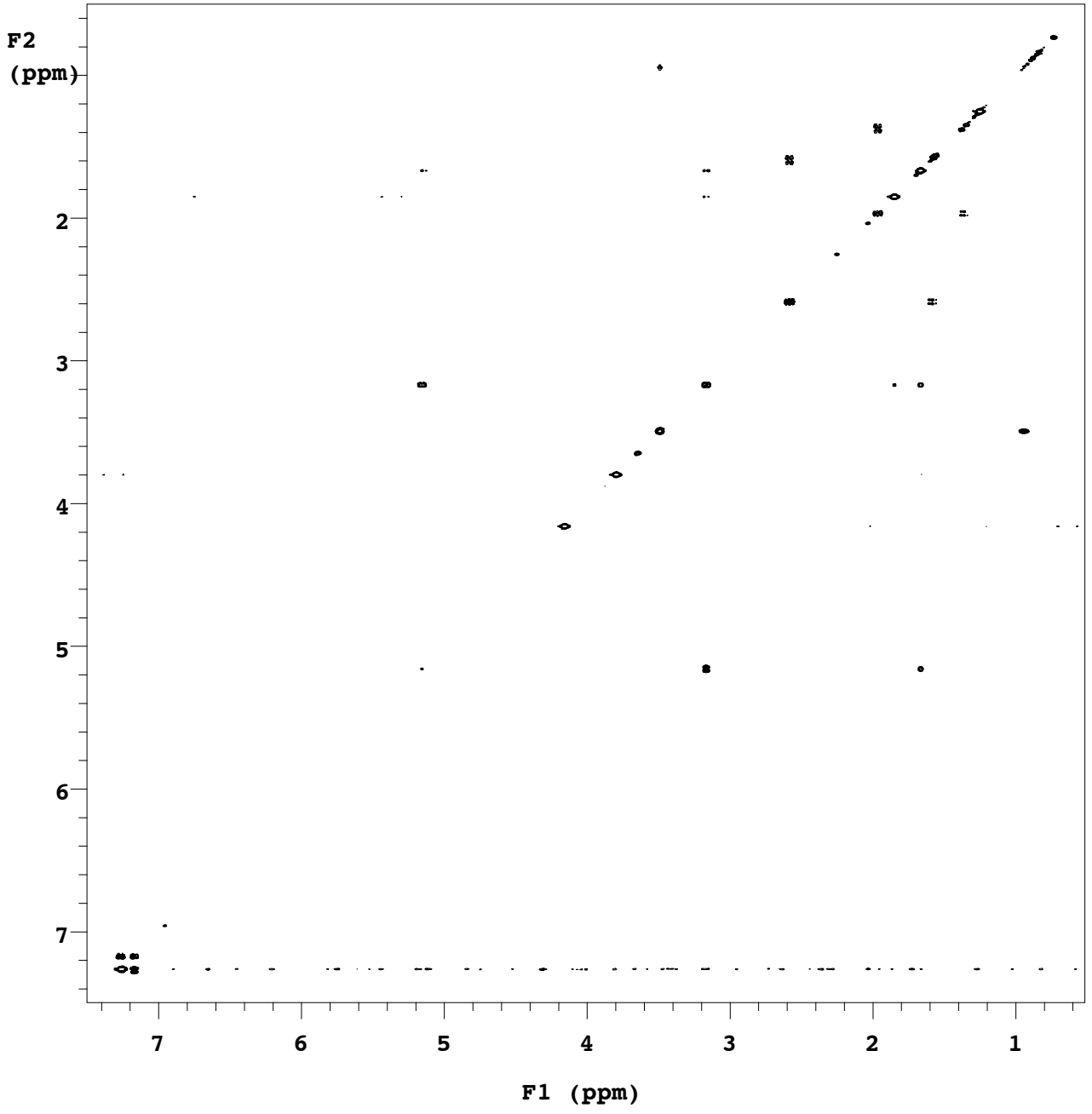


Figure S 3. HSQC spectrum (CDCl3, 1H 600 MHz) of lehualide E (5).

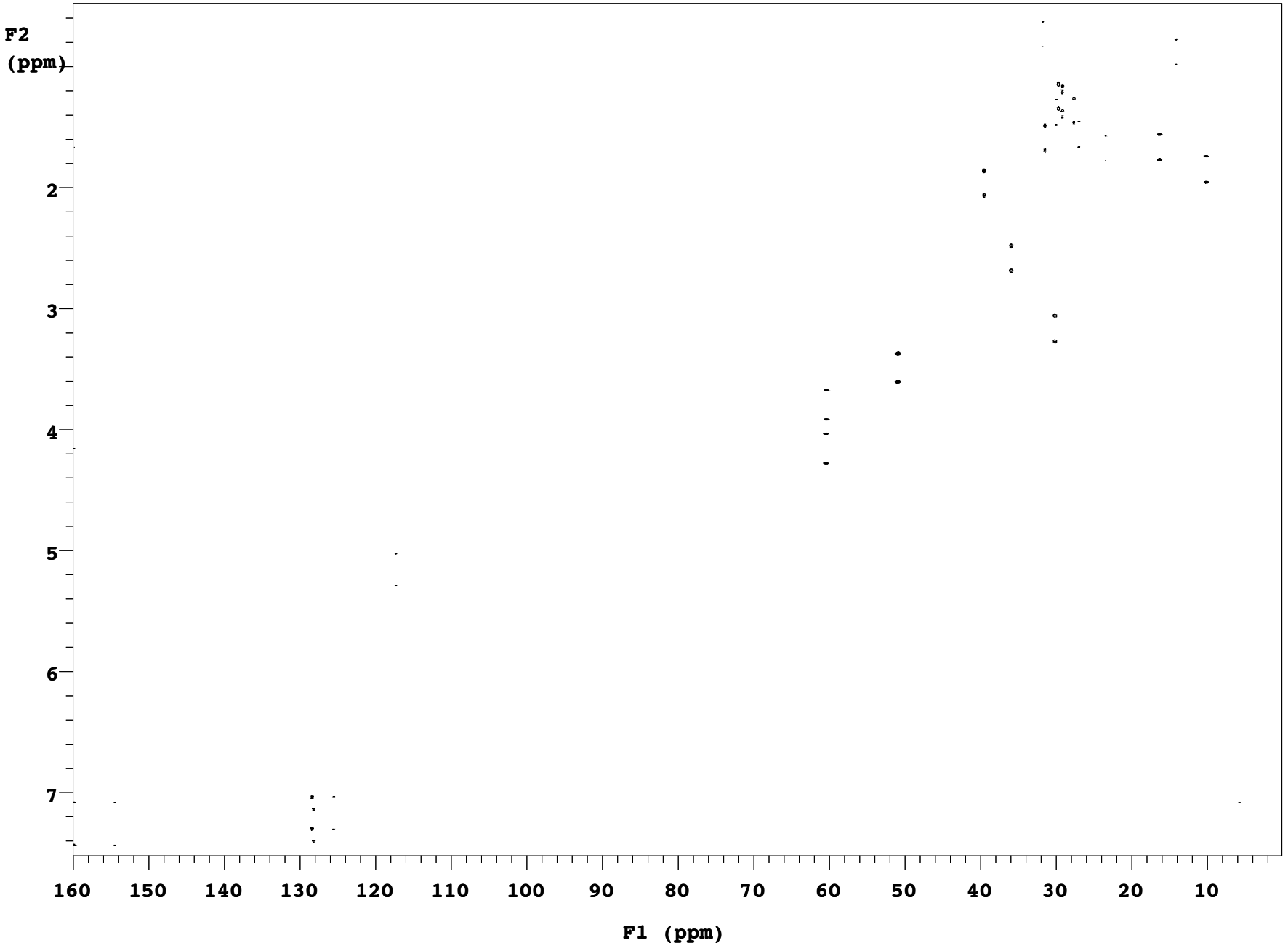


Figure S 4. HMBC spectrum (CDCl3, 1H 600 MHz) of lehualide E (5).

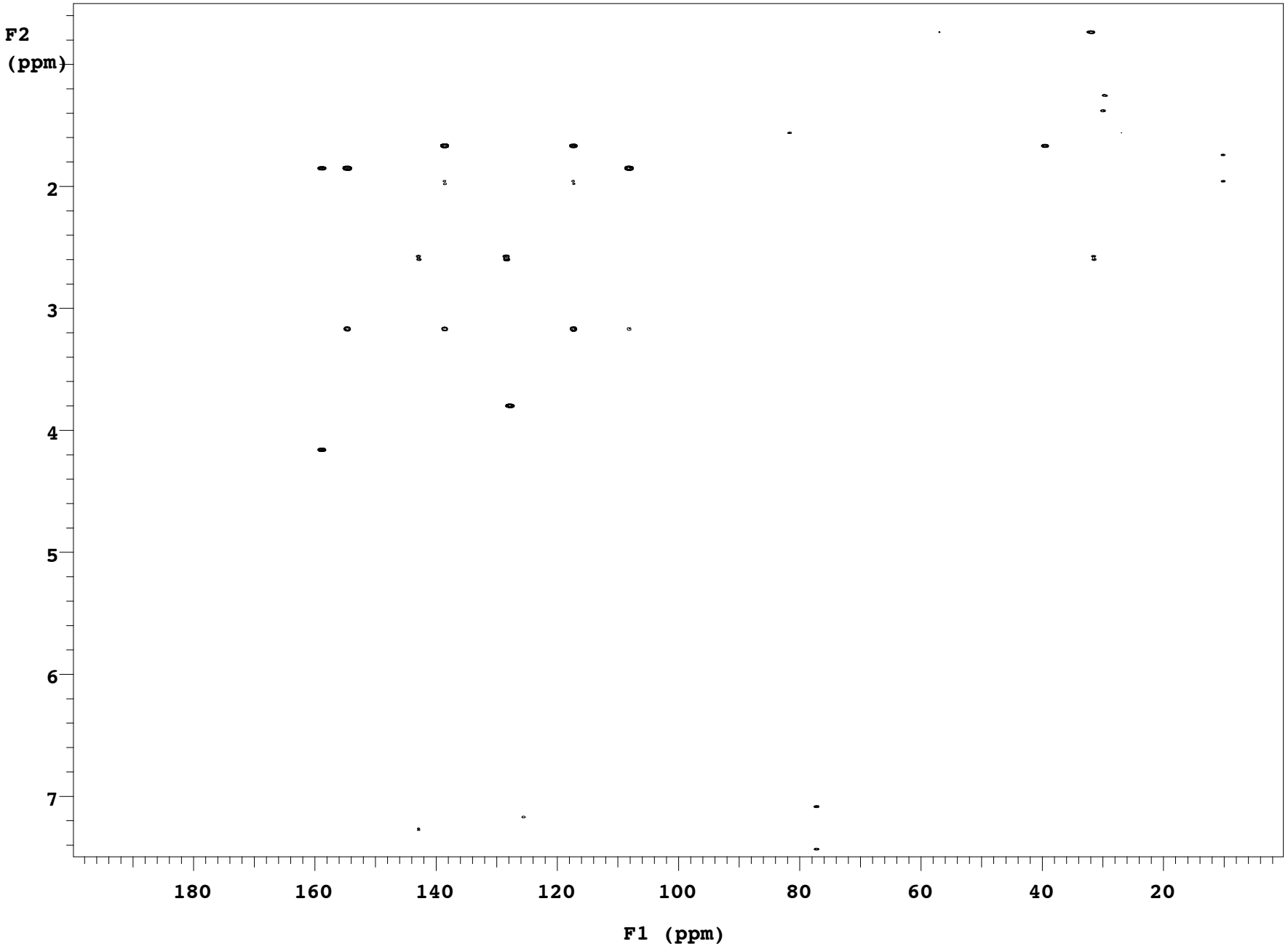
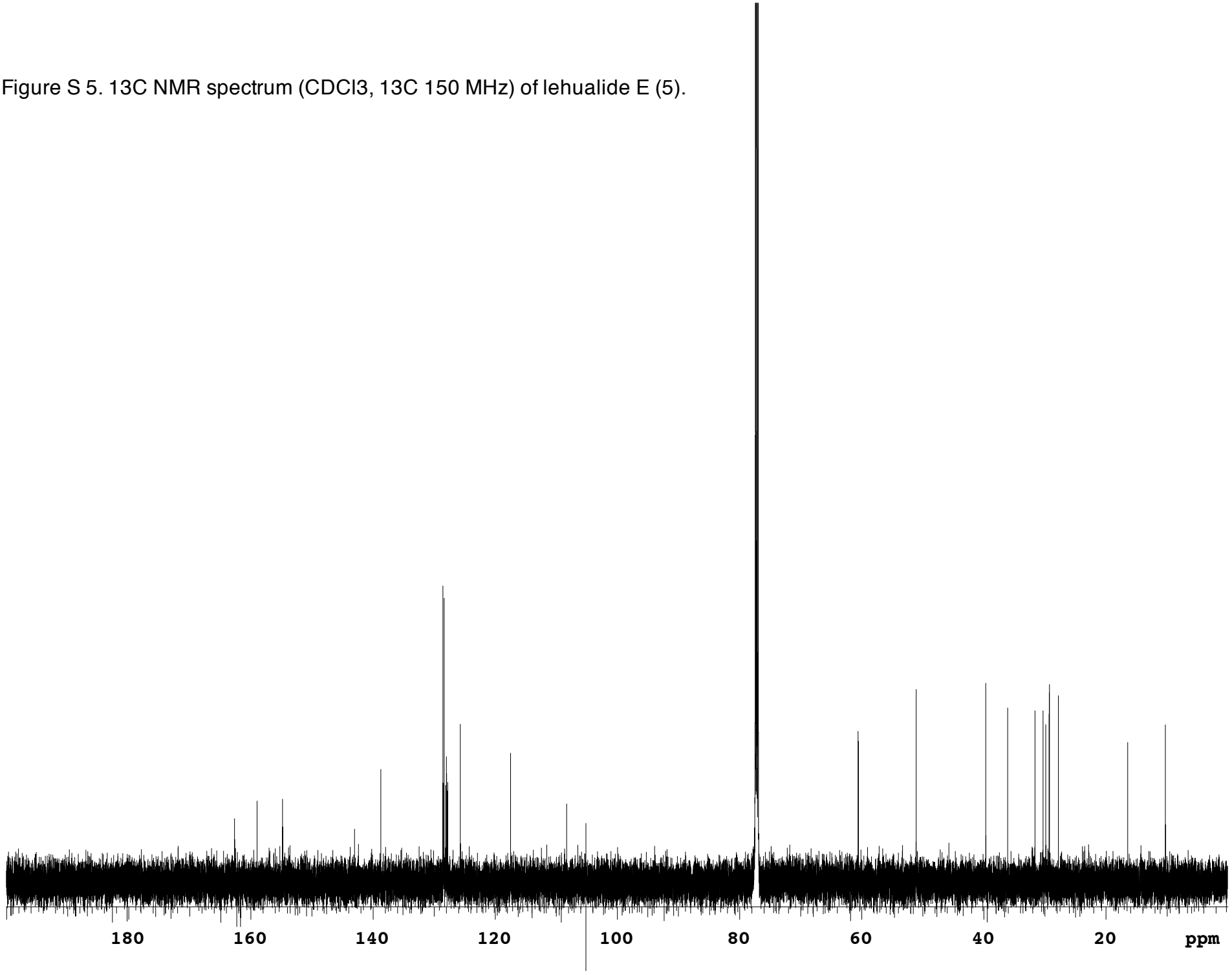


Figure S 5. 13C NMR spectrum (CDCl3, 13C 150 MHz) of lehualide E (5).



Lehualide F (**6**)

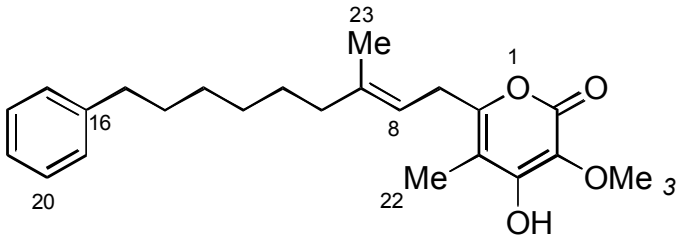


Table S 2. NMR Spectroscopic Data ($CDCl_3$, ^1H 600 MHz; ^{13}C 150 MHz) of Lehualide F (**6**).

	6				
position	**δ_C , mult**	**δ_H (*J*, Hz)**	**COSY**	**HMBC (H → C)**	**NOE[a]**
2	160.3, C				
3	125.0, C				
OCH_3 3	59.8, CH_3	3.90		3	
4	157.9, C				
5	105.6, C				
6	157.3, C				
7	30.2, CH_2	3.20, d (7.2)	22[b]	6; 8; 5[b]	22; 23
8	117.2, CH	5.17, t (7.0)	7; 23[b]	7; 9; 23	10
9	139.0, C				
10	39.7, CH_2	1.97, t (8.4)	11	9; 11	8
11	27.8, CH_2	1.38, quin (7.6)	10; 12	8; 9; 11; 23	23
12	29.29, CH_2	1.32, quin (8.0)	11; 13	10; 11; 13	
13	29.26, CH_2	1.24 – 1.29, m			
14	31.5, CH_2	1.59, quin (8.0)	13; 15	13; 15	
15	36.1, CH_2	2.57, t (7.2)	13; 14	14; 15; 16	
16	143.0, C				
17	128.5, CH	7.17, d (8.2)	18	19; 21	
18	128.4, CH	7.22, t (7.7)	17; 19	16; 20	
19	125.6, CH	7.16, t (6.0)	18; 20	17; 21	
20	128.4, CH	7.22, t (7.7)	19; 21	16; 18	
21	128.5, CH	7.17, d (8.2)	20	17; 19	
22	9.4, CH_3	1.96, s	7[b]	5; 4; 6	7
23	16.3, CH_3	1.68, s		8; 9; 10	11; 7

[a] Selected correlations

[b] Weak correlation

Figure S 6. 1H NMR spectrum (CDCl3, 1H 600 MHz) of lehualide F (6).

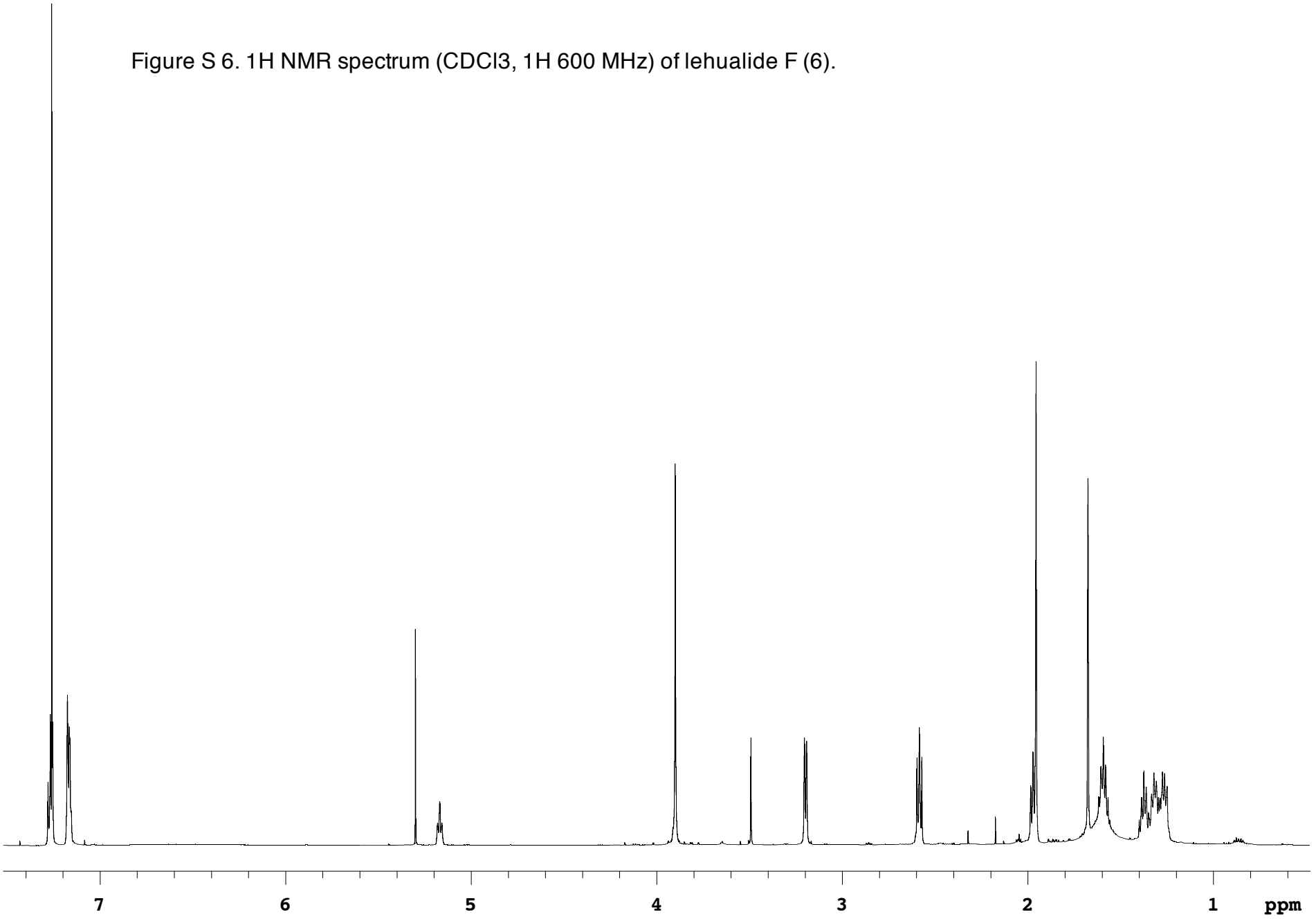


Figure S 7. COSY spectrum (CDCl3, 1H 600 MHz) of lehualide F (6).

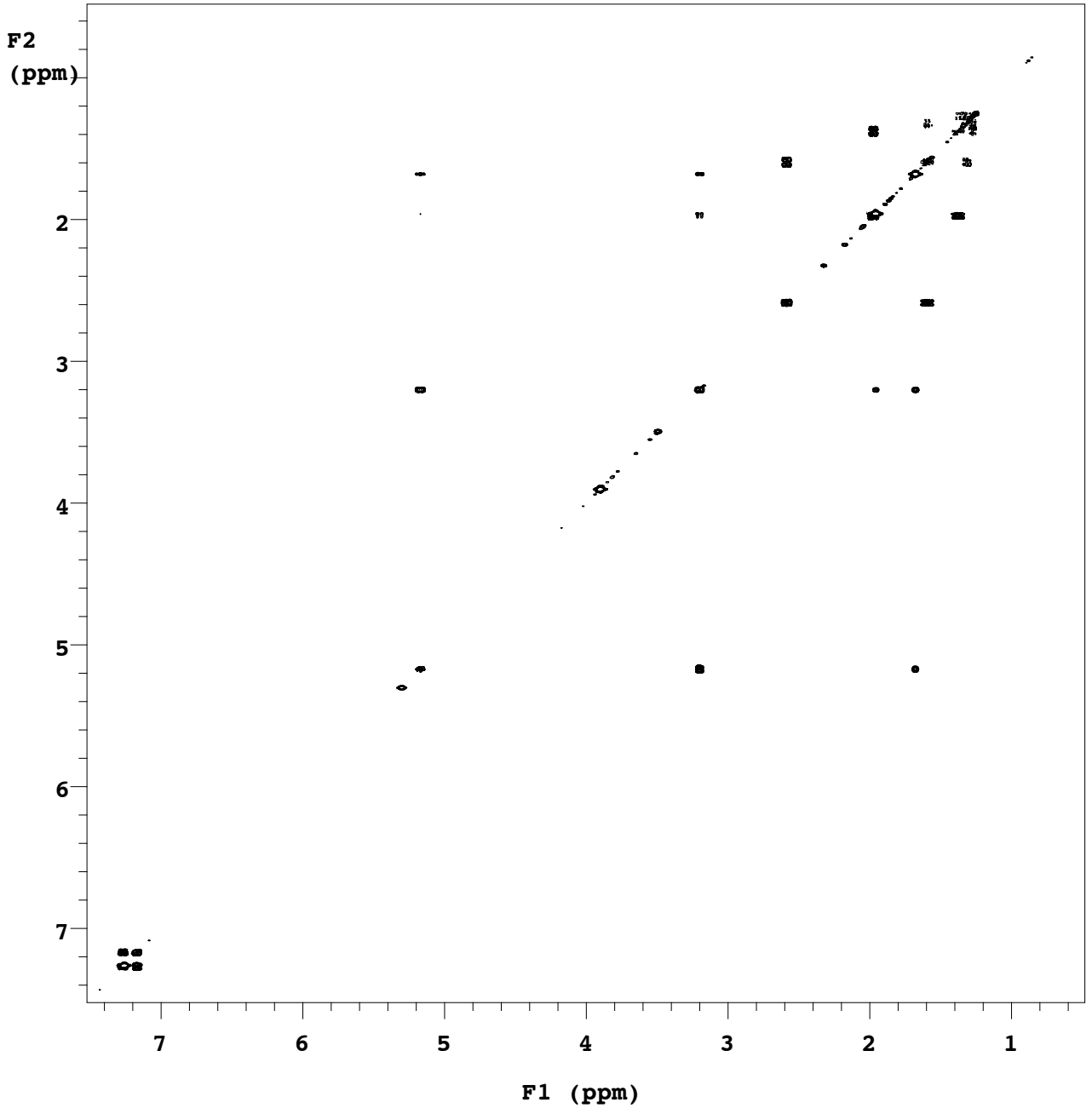


Figure S 8. HSQC spectrum (CDCl3, 1H 600 MHz) of lehualide F (6).

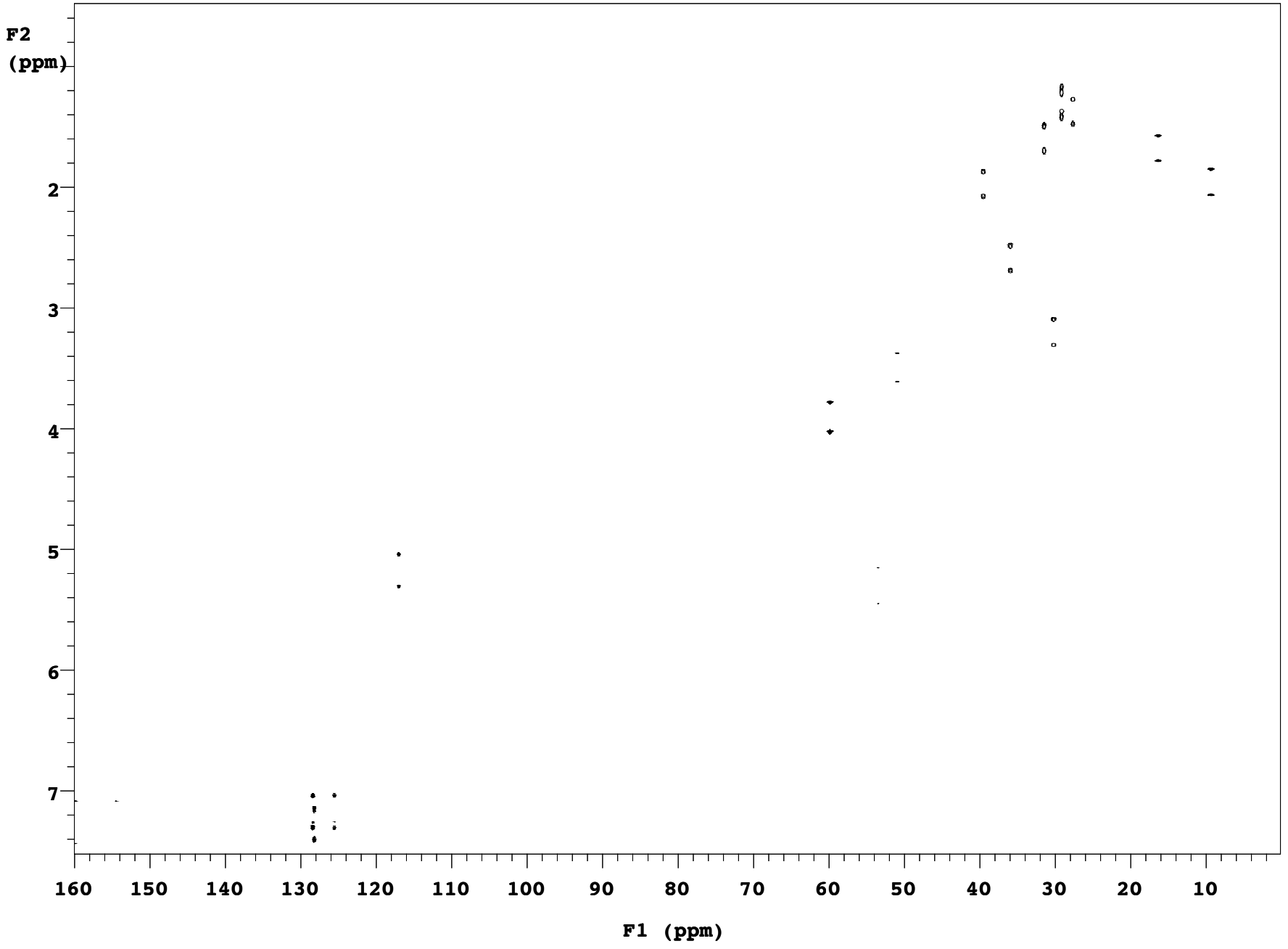


Figure S 9. HMBC spectrum (CDCl3, 1H 600 MHz) of lehualide F (6).

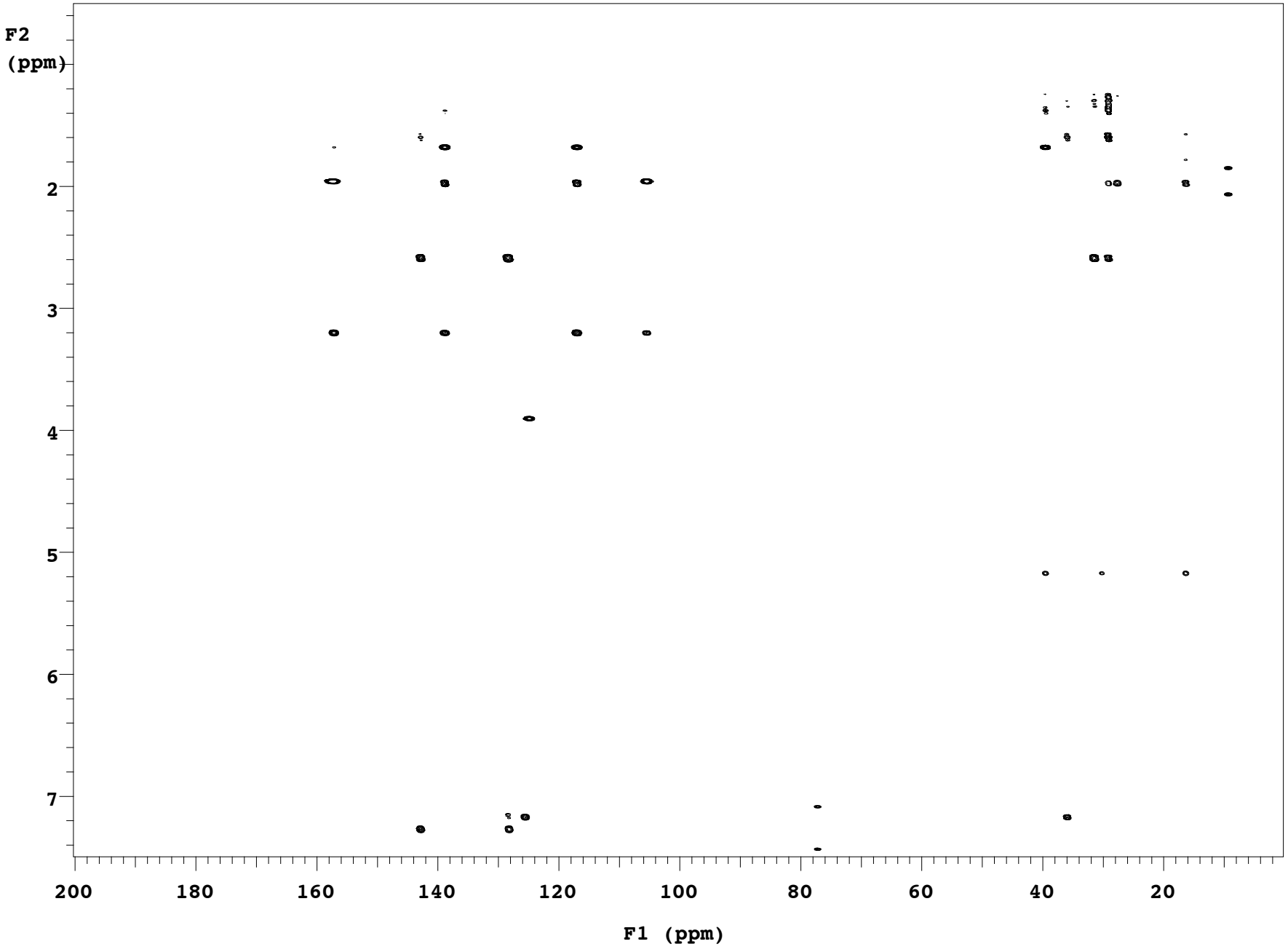
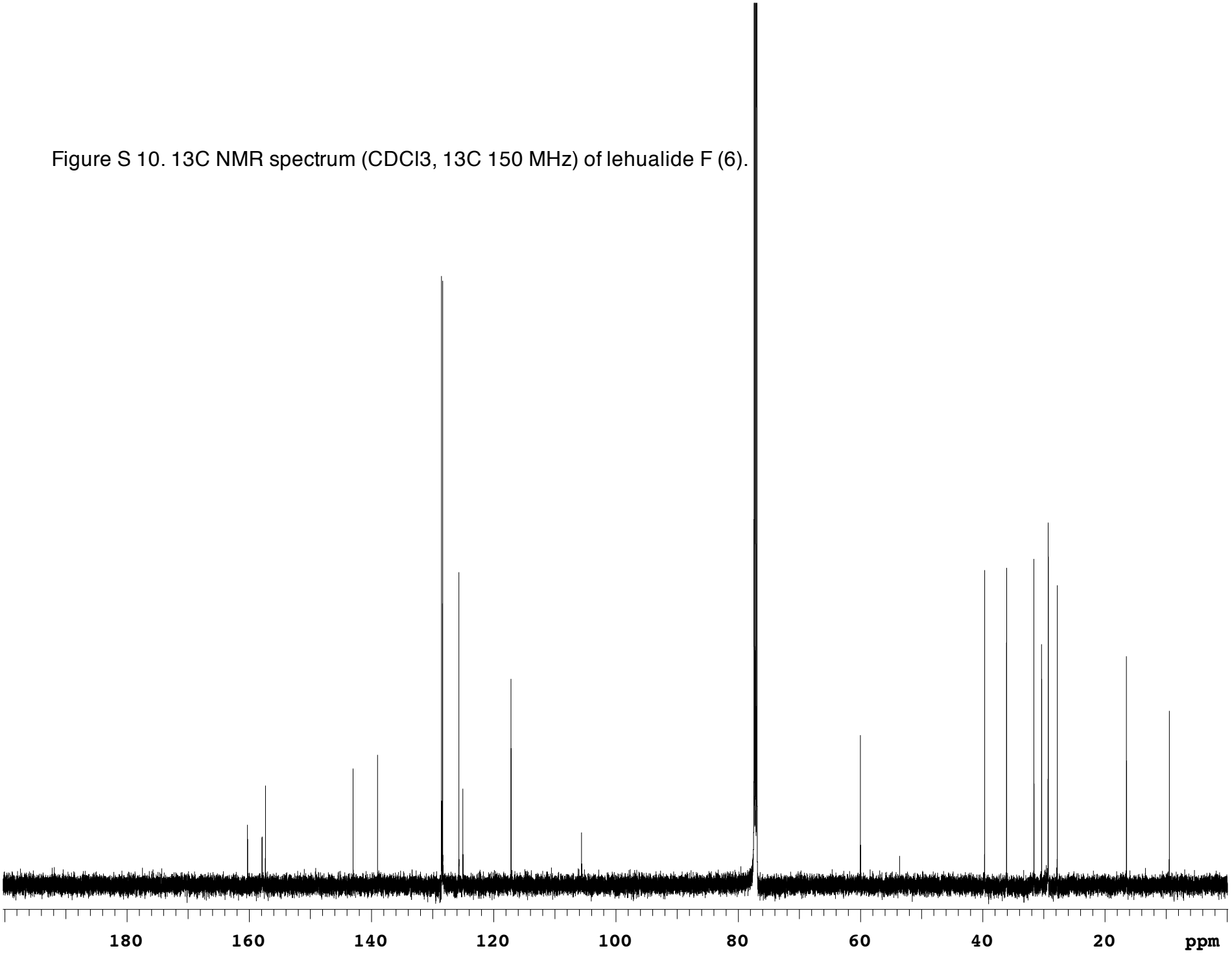


Figure S 10. 13C NMR spectrum (CDCl3, 13C 150 MHz) of lehualide F (6).



Lehualide G (**7**)

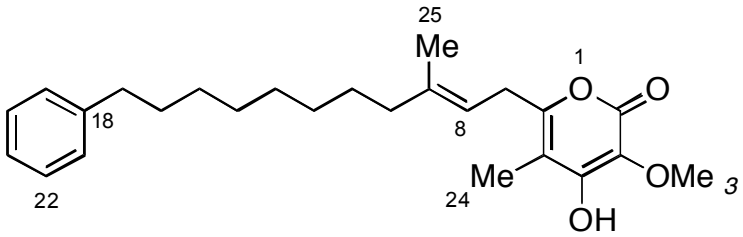


Table S 3. NMR Spectroscopic Data ($CDCl_3$, ^1H 600 MHz; ^{13}C 150 MHz) of Lehualide G (**7**).

			7		
position	**δ_C , mult**	**δ_H (*J*, Hz)**	**COSY**	**HMBC (H → C)**	**NOE[a]**
2	160.4, C				
3	125.0, C				
OCH_3 3	60.0, CH_3	3.86, s		3	
4	158.0, C				
5	105.7, C				
6	157.3, C				
7	30.3, CH_2	3.21, d (7.0)	24[b]	6; 8	24; 25
8	117.1, CH	5.16, t (7.0)	7; 25[b]	7; 25; 6[b]	10
9	139.1, C				
10	39.7, CH_2	1.97, t (7.4)	11; 25	8;11; 25;	8
11	27.8, CH_2	1.36, quin (7.1)	10; 12	9; 10; 12	25
12	29.4, CH_2	1.20 – 1.33, m			
13	29.55, CH_2	1.20 – 1.33, m			
14	29.58, CH_2	1.20 – 1.33, m			
15	29.45, CH_2	1.20 – 1.33, m			
16	31.7, CH_2	1.59, quin (6.9)	15; 17	15; 17	
17	36.1, CH_2	2.61, t (7.8)	16	16; 18; 19; 23	
18	143.1, C				
19	128.5, CH	7.17, d (7.4)	20	21; 23	
20	128.3, CH	7.27, t (7.3)	19; 21	18; 22	
21	125.7, CH	7.16, t (6.3)	20; 22	19; 23	
22	128.3, CH	7.27, t (7.3)	21; 23	18; 20	
23	128.5, CH	7.17, d (7.4)	22	19; 21	
24	9.5, CH_3	1.96, s	7[b]	5; 4; 6	7
25	16.5, CH_3	1.68, s		8; 9; 10	7; 11
OH		6.50, bs			

[a] Selected correlations

Figure S 11. 1H NMR spectrum (CDCl3, 1H 600 MHz) of lehualide G (7).

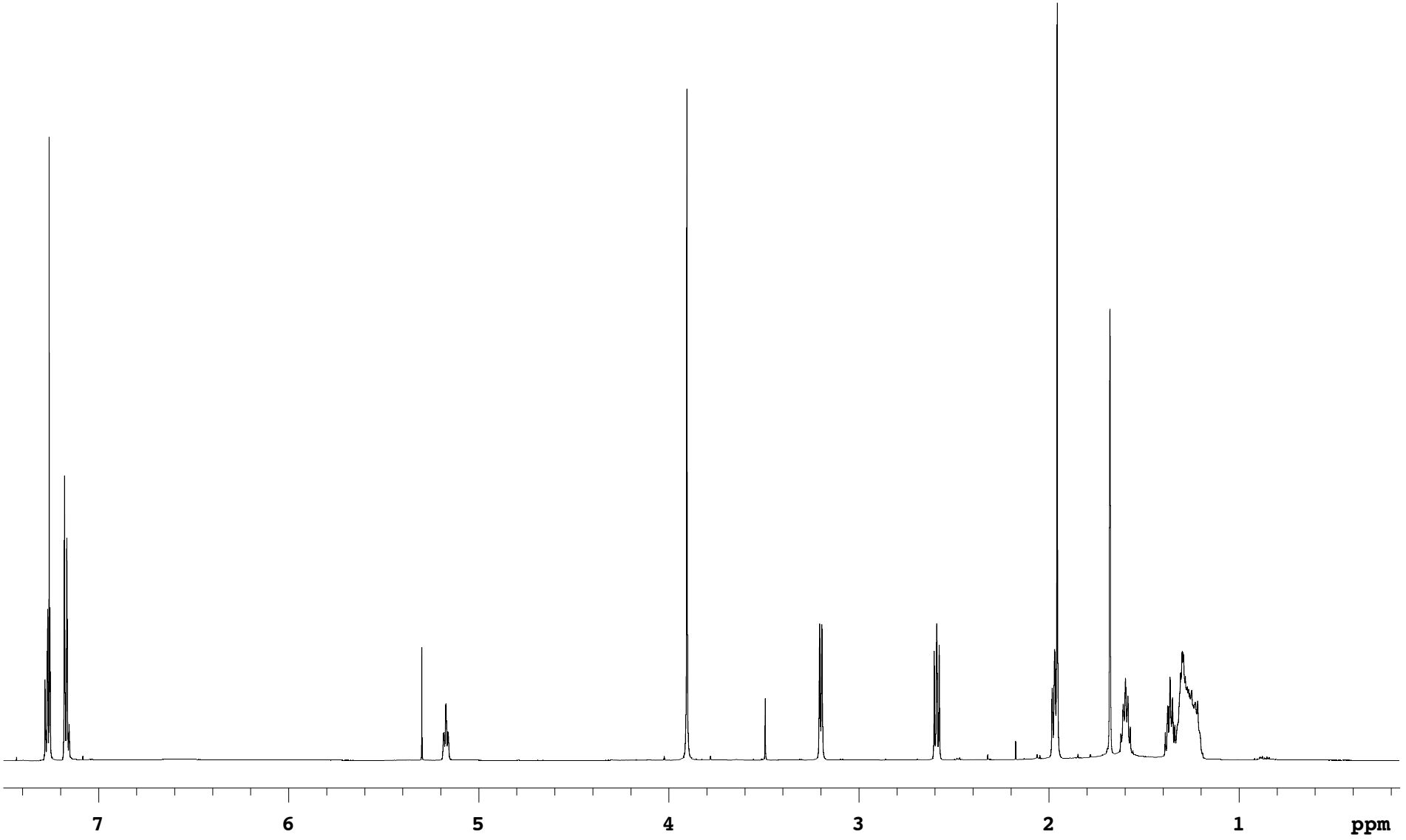


Figure S 12. COSY spectrum (CDCl3, 1H 600 MHz) of lehualide G (7).

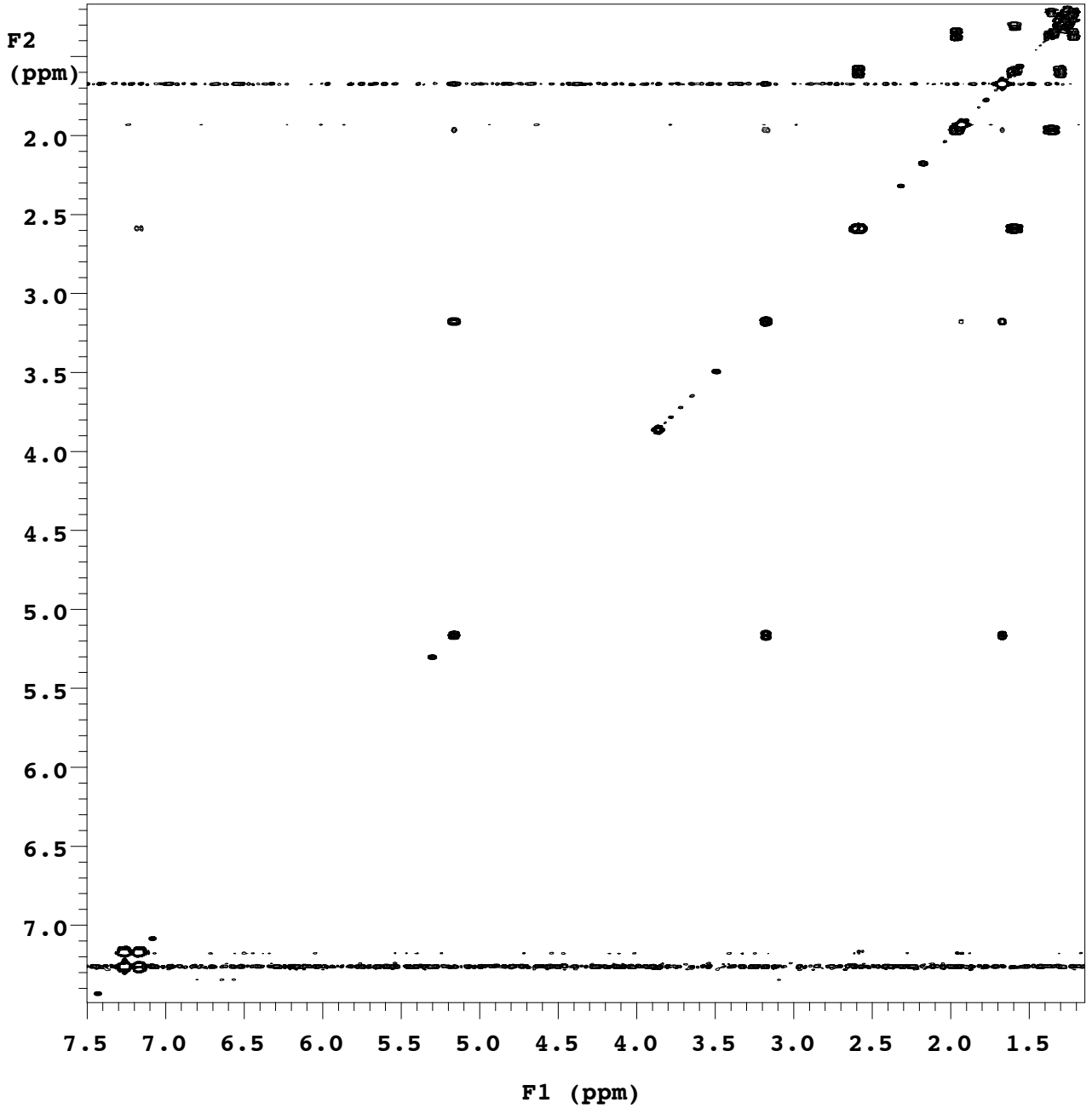


Figure S 13. HSQC spectrum (CDCl3, 1H 600 MHz) of lehualide G (7).

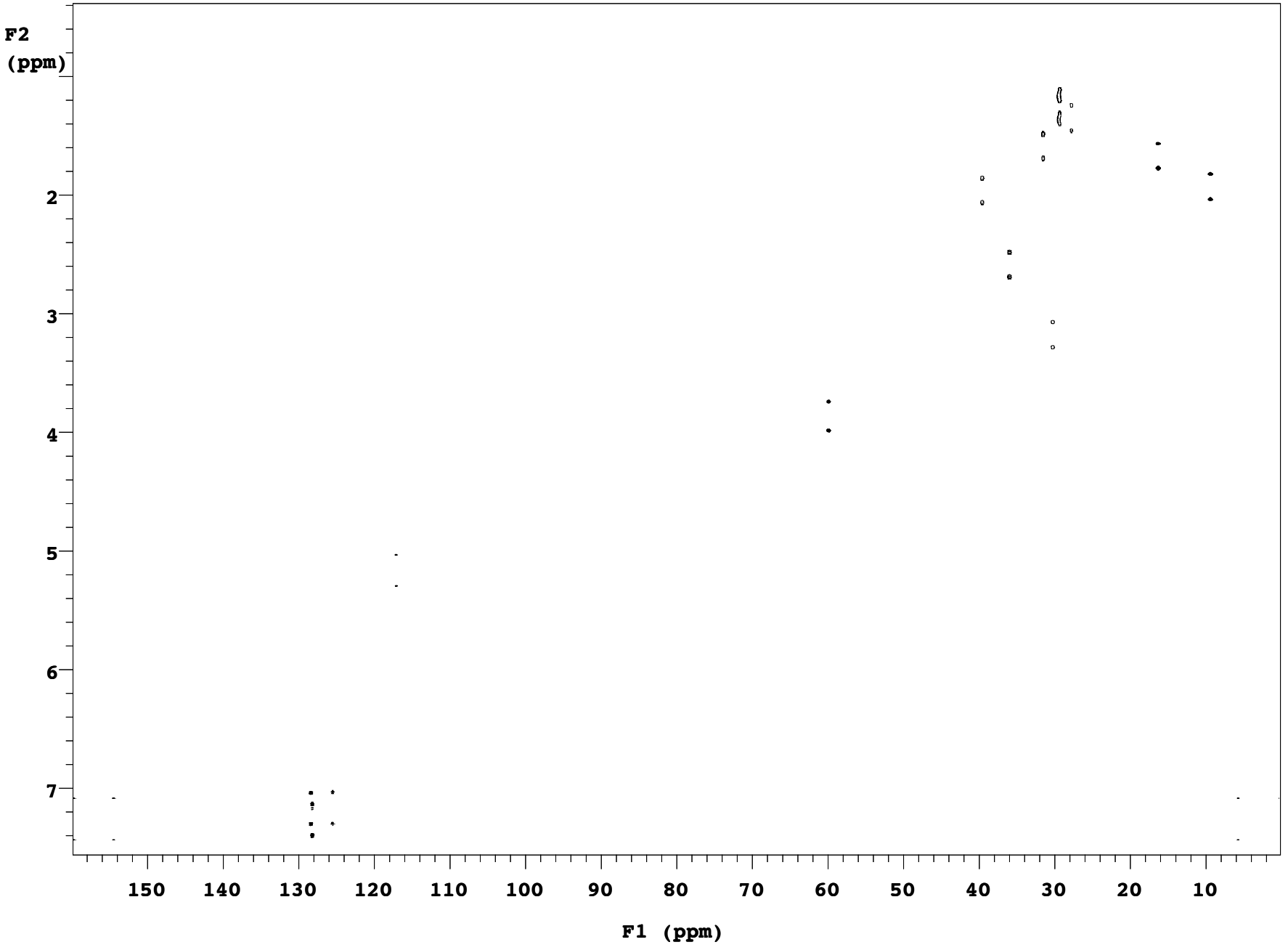


Figure S 14. HMBC spectrum (CDCl3, 1H 600 MHz) of lehualide G (7).

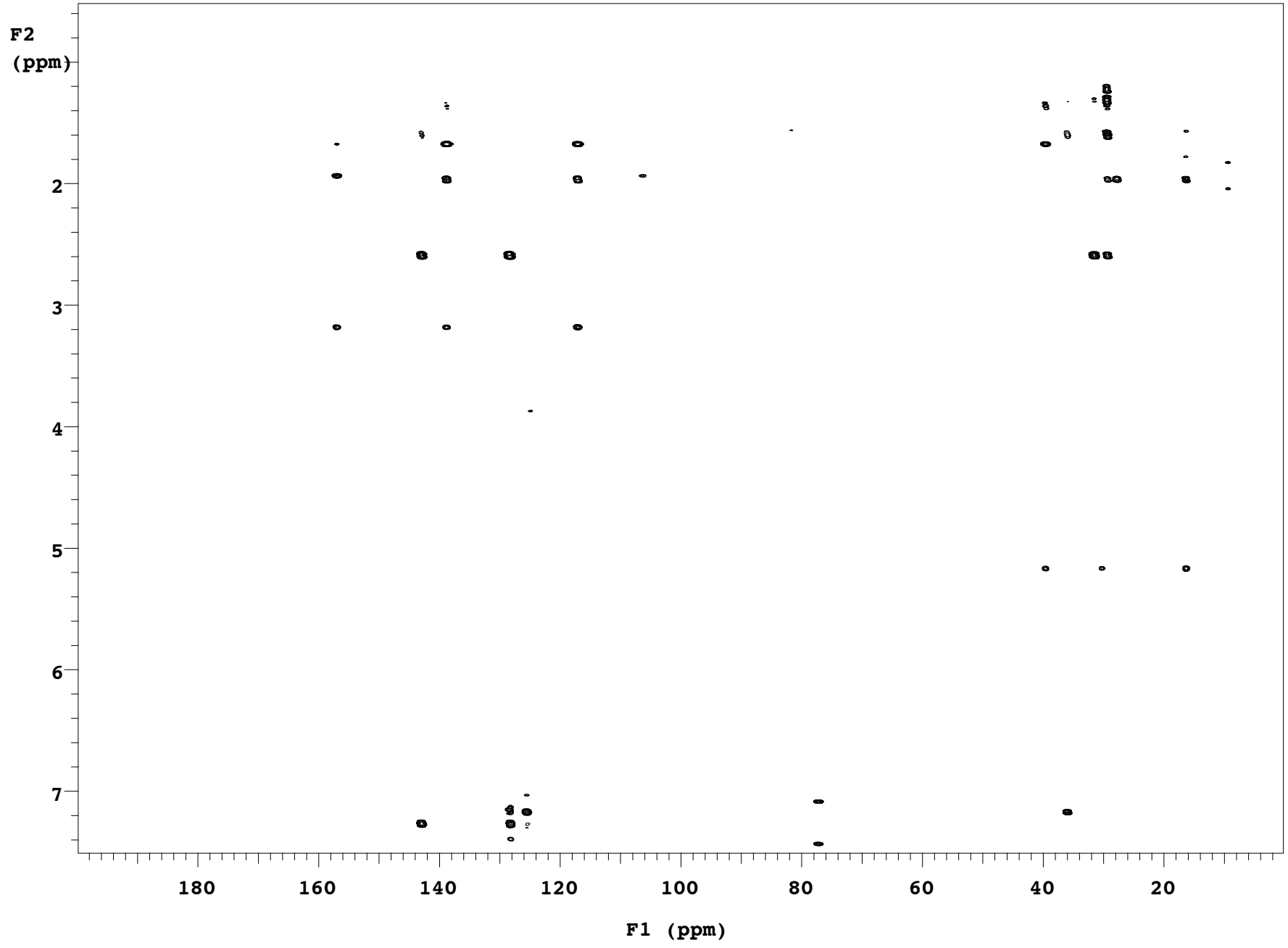


Figure S 15. 13C NMR spectrum (CDCl3, 13C 150 MHz) of lehualide G (7).

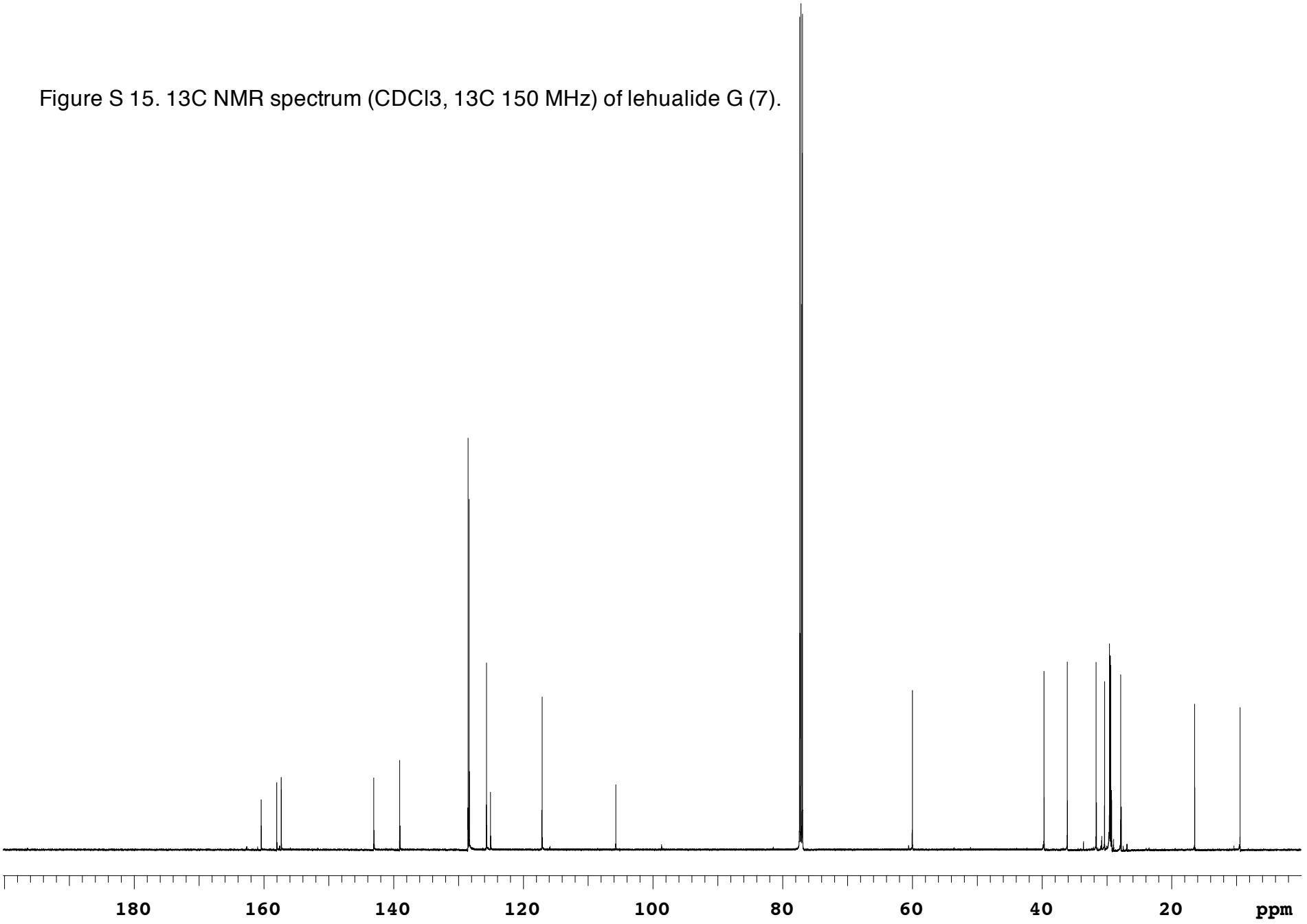


Figure S 16. 1H NMR spectrum (CD3OD, 1H 600 MHz) of lehualide G (7).

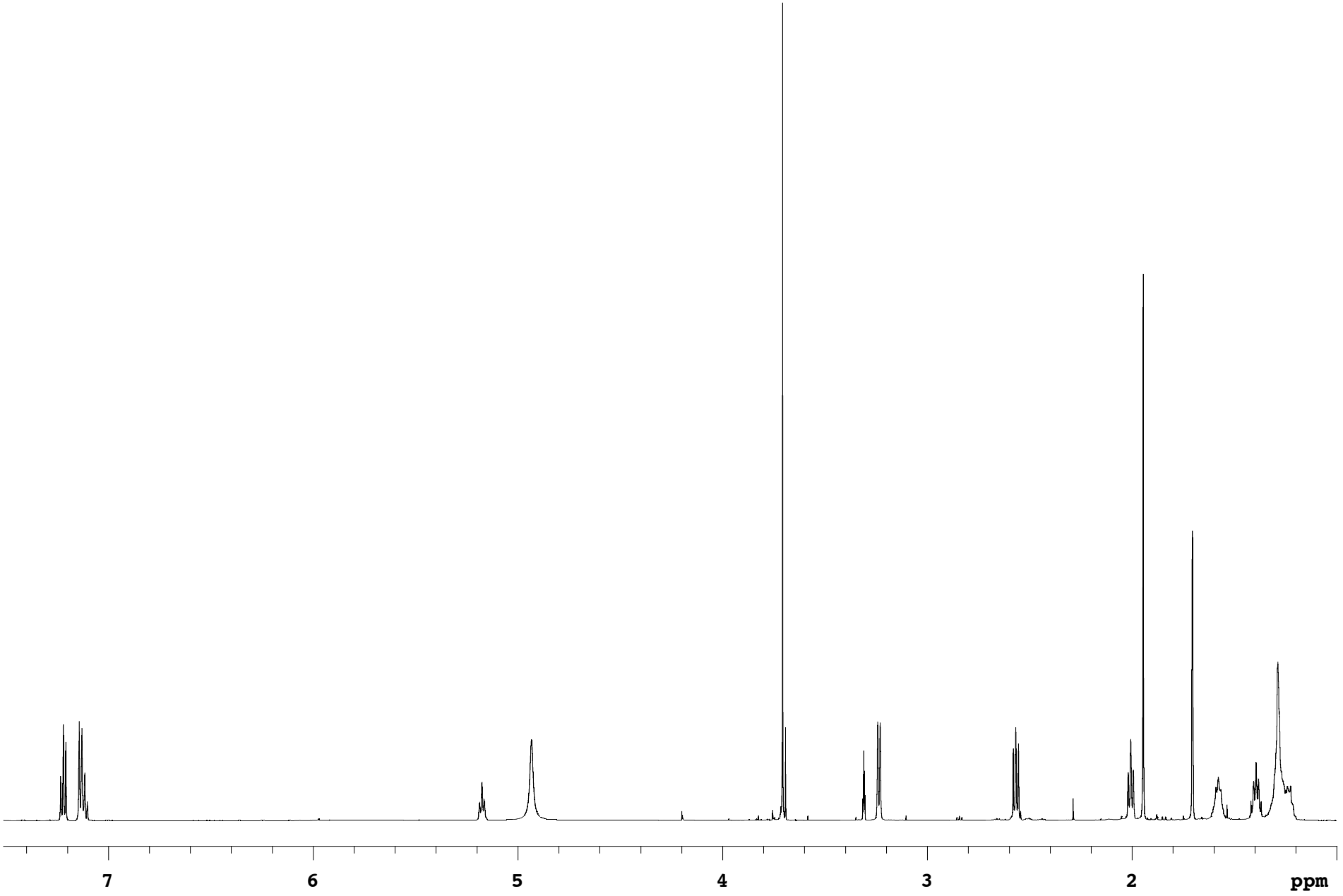


Figure S 17. COSY spectrum (CD3OD, 1H 600 MHz) of lehualide G (7).

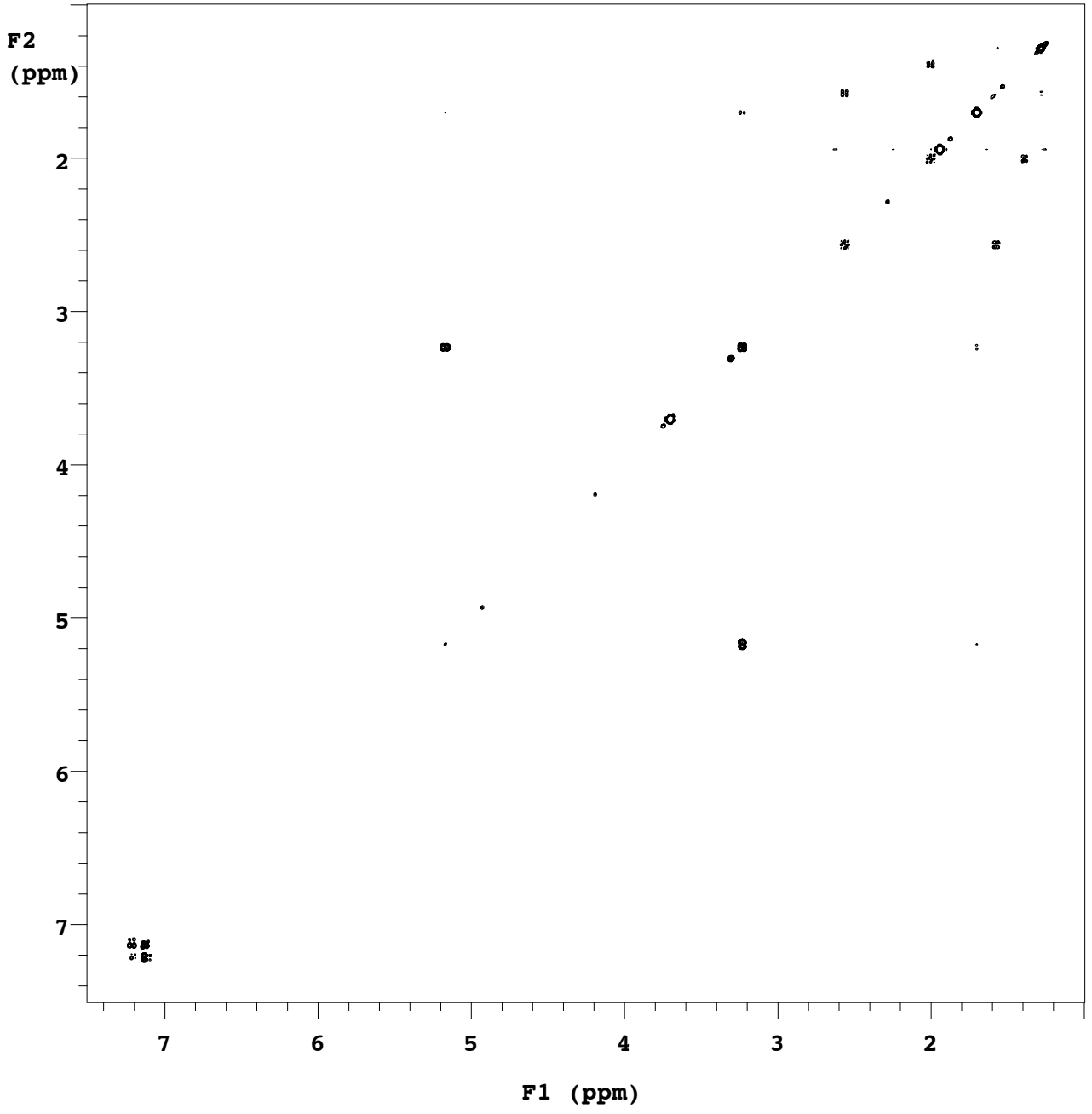


Figure S 18. HSQC spectrum (CD3OD, 1H 600 MHz) of lehualide G (7).

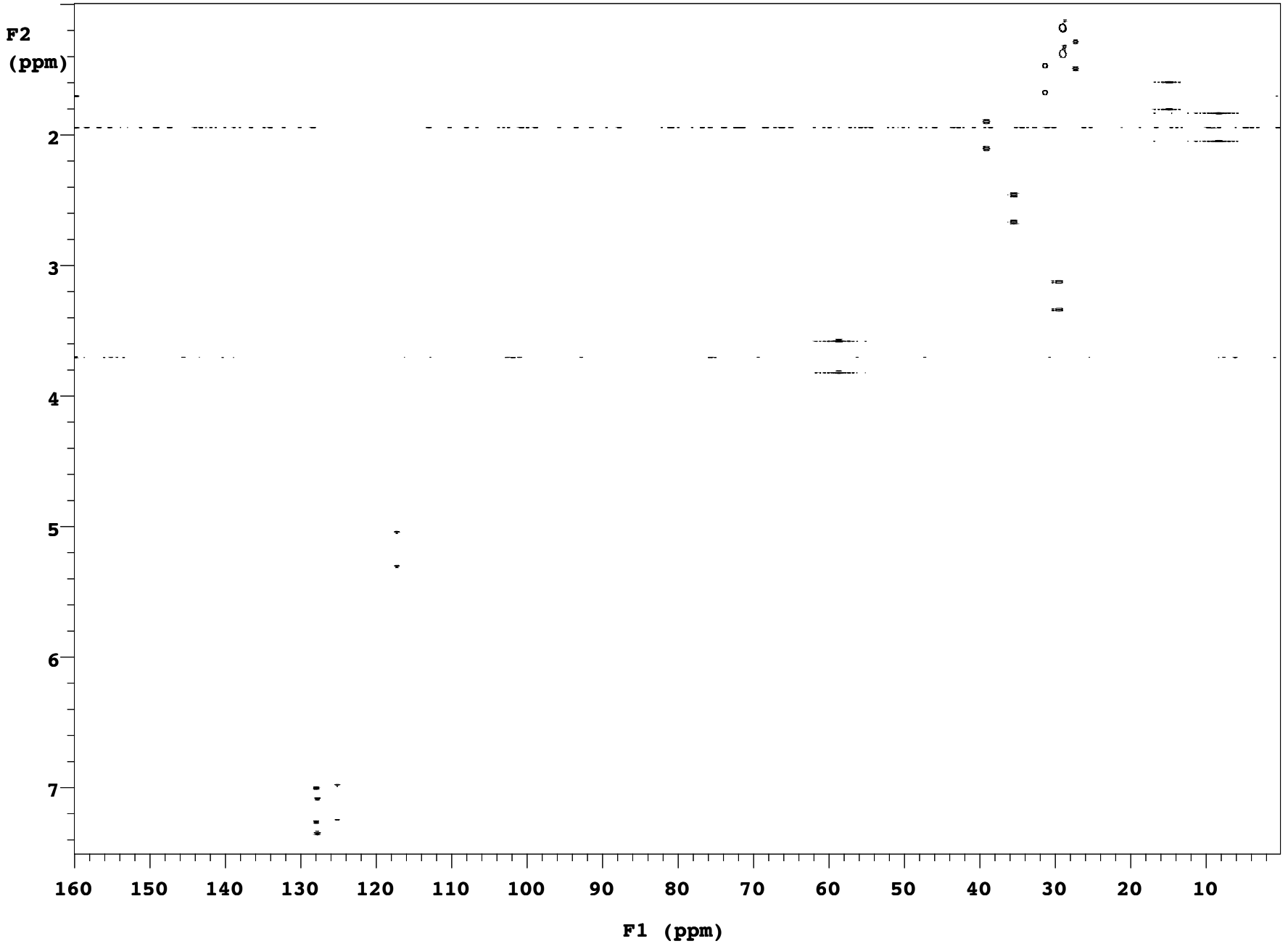


Figure S 19. band-selective HSQC-TOCSY spectrum (CD3OD, 1H 600 MHz) of lehualide G (7).

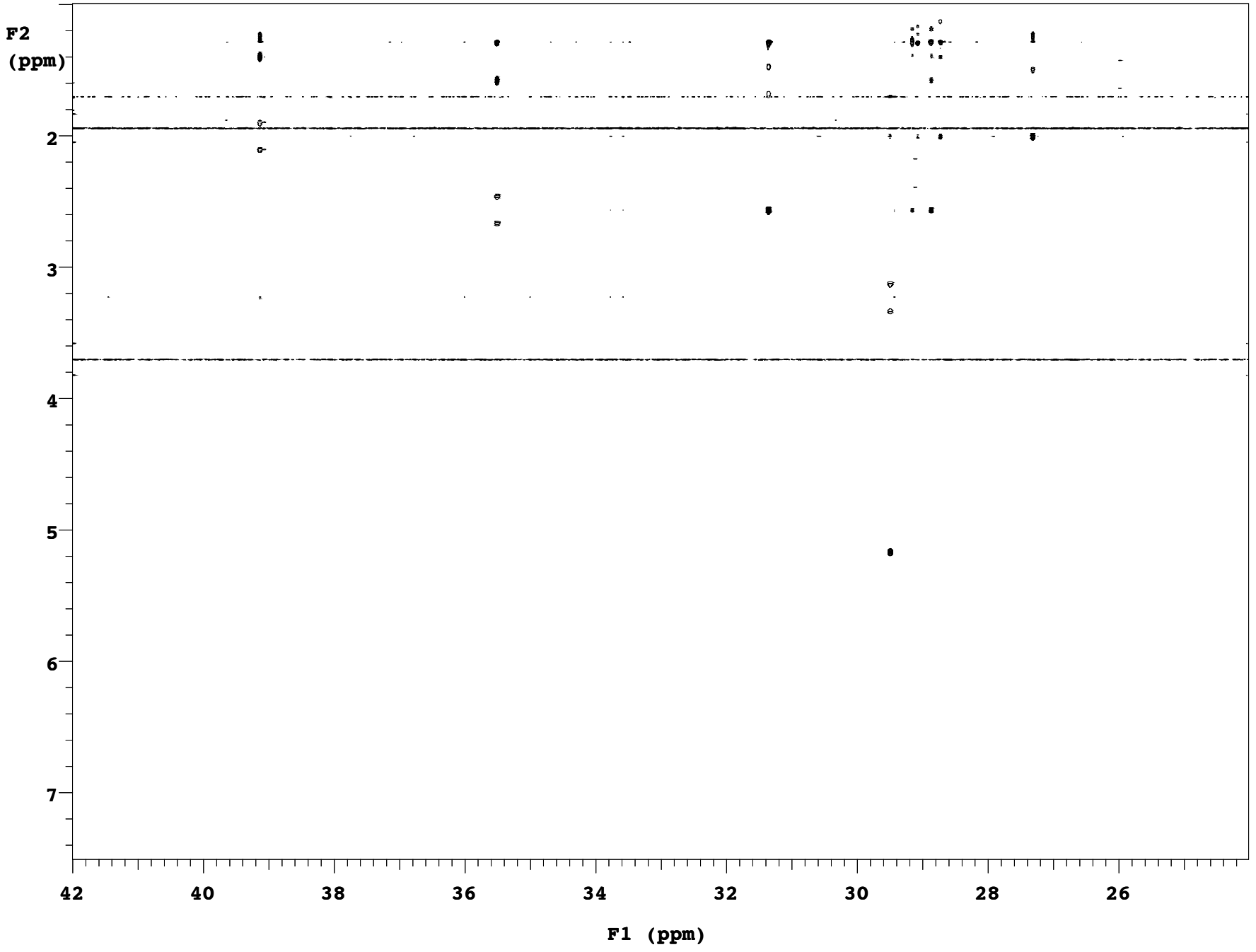


Figure S 20. HMBC spectrum (CD3OD, 1H 600 MHz) of lehualide G (7).

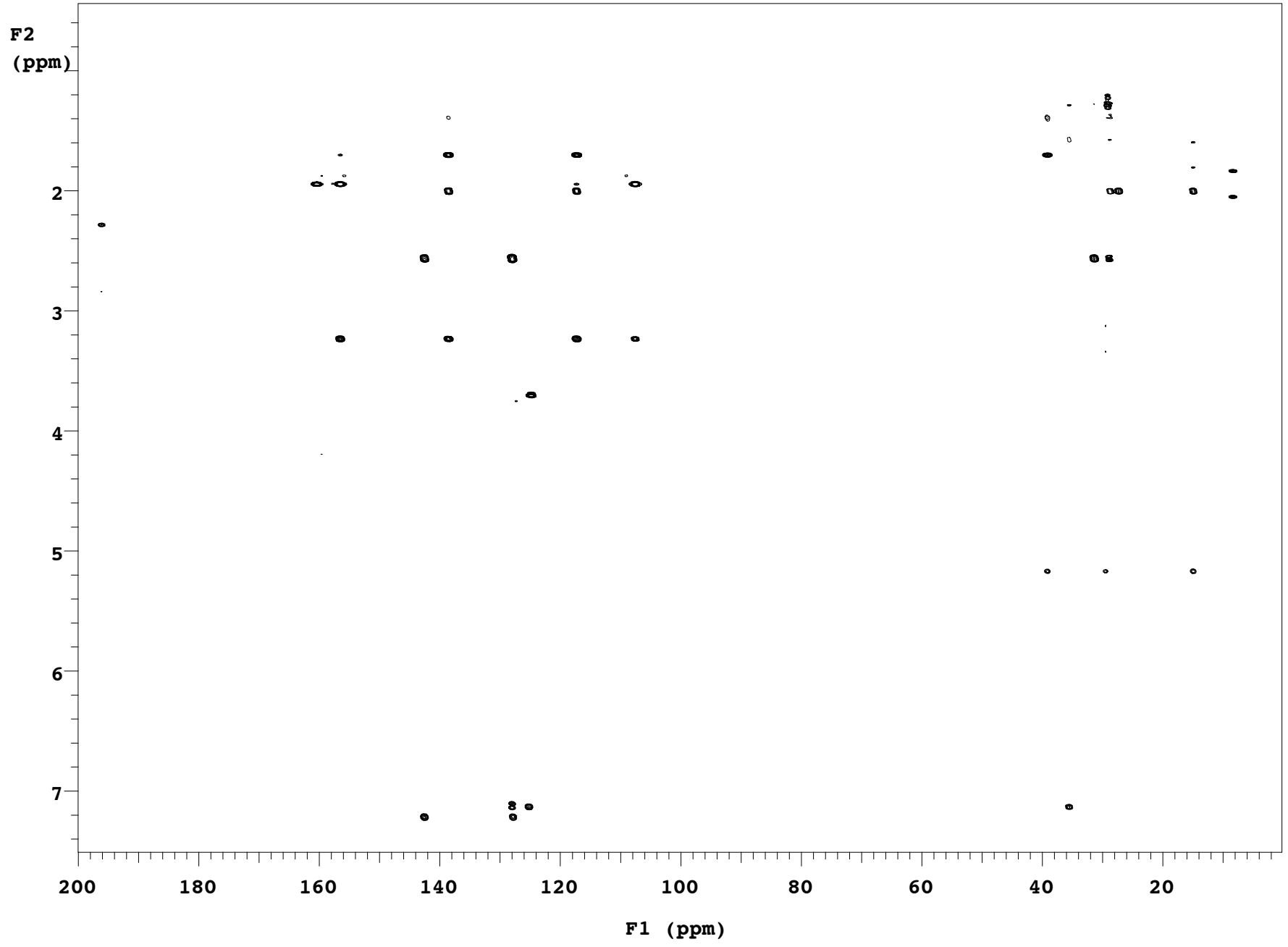
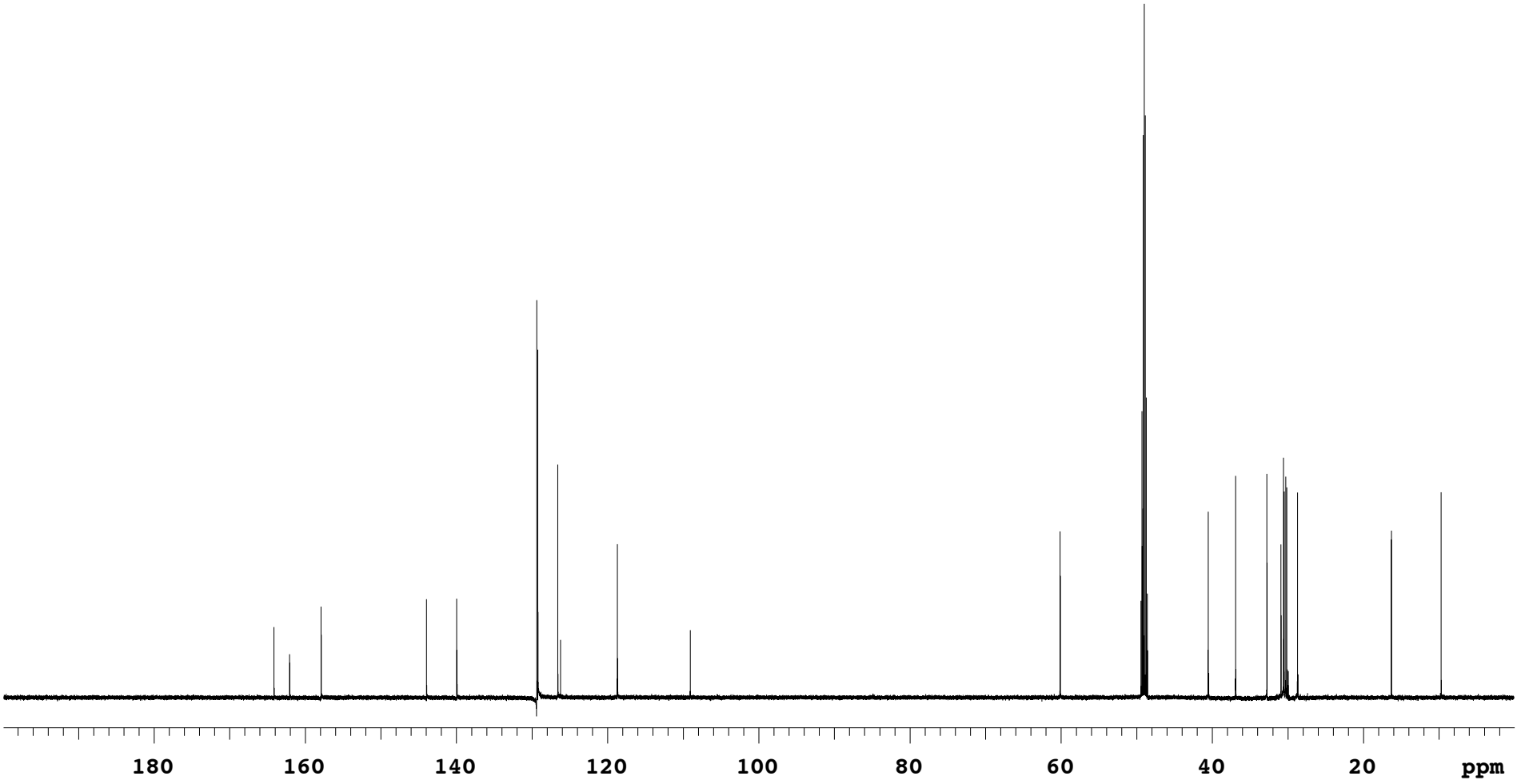


Figure S 21. 13C NMR spectrum (CD3OD, 13C 150 MHz) of lehualide G (7).



Lehualide H (**8**)

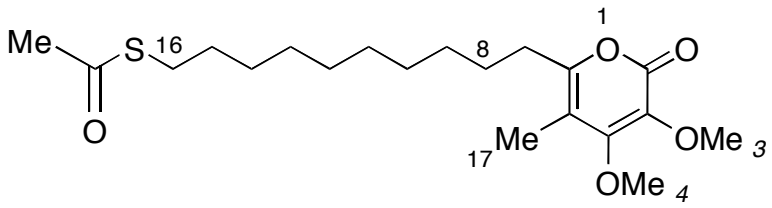


Table S 4. NMR Spectroscopic Data ($CDCl_3$, ^1H 600 MHz; ^{13}C 150 MHz) of Lehualide H (**8**).

		8			
position	**δ_C , mult**	**δ_H (*J*, Hz)**	**COSY**	**HMBC (H → C)**	**NOE[a]**
2	162.7, C				
3	127.9, C				
OCH_3 3	60.4, CH_3	3.81, s		3	*O*CH_3 4
4	158.9, C				
OCH_3 4	60.6, CH_3	4.16, s		4	*O*CH_3 3;
5	108.5, C				
6	155.9, C				
7	30.9, CH_2	2.44, t (7.7)	8; 17[b]	8; 6; 5[b]	17
8	27.5, CH_2	1.58, quin (7.5)	7; 9	7; 9; 6[b]	
9	29.3, CH_2	1.28, m			
10	29.4, CH_2	1.27, m			
11	29.54, CH_2	1.25, m			
12	29.55, CH_2	1.25, m			
13	29.48, CH_2	1.23, m			
14	28.9, CH_2	1.35, m	15; 13	15; 16; 13	
15	29.48, CH_2	1.55, t (7.2)	14; 16	14; 16; *S***C=O**CH_3	
16	29.2, CH_2	2.86, t (7.3)			
*S***C=O**CH_3	196.3, C				
*S*C=O**CH_3**	30.8, CH_3	2.35, s	16[b]	*S***C=O**CH_3; 16	
17	10.5, CH_3	1.84, s	7[b]	5; 4; 6	*O*CH_3 4; 7

[a] Selected correlations

[b] Weak correlation

Figure S 22. 1H NMR spectrum (CDCl3, 1H 600 MHz) of lehualide H (8).

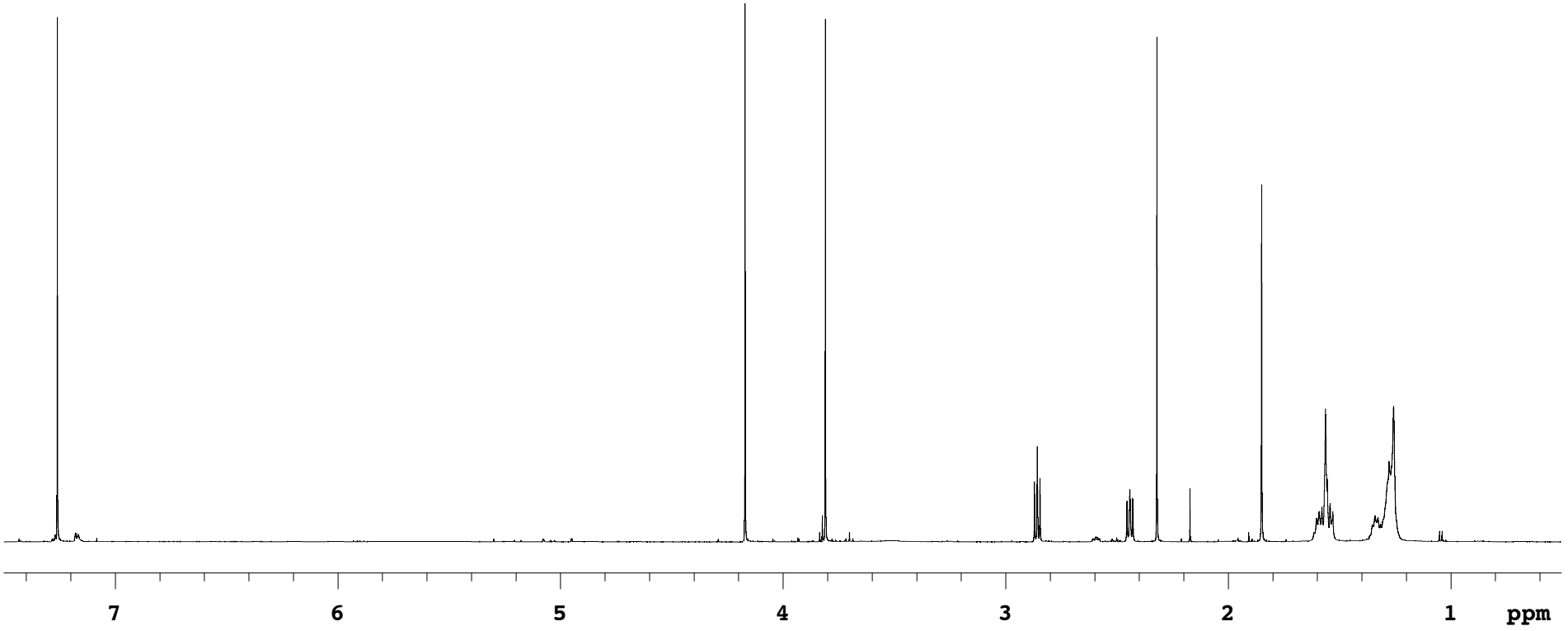


Figure S 23. COSY spectrum (CDCl3, 1H 600 MHz) of lehualide H (8).

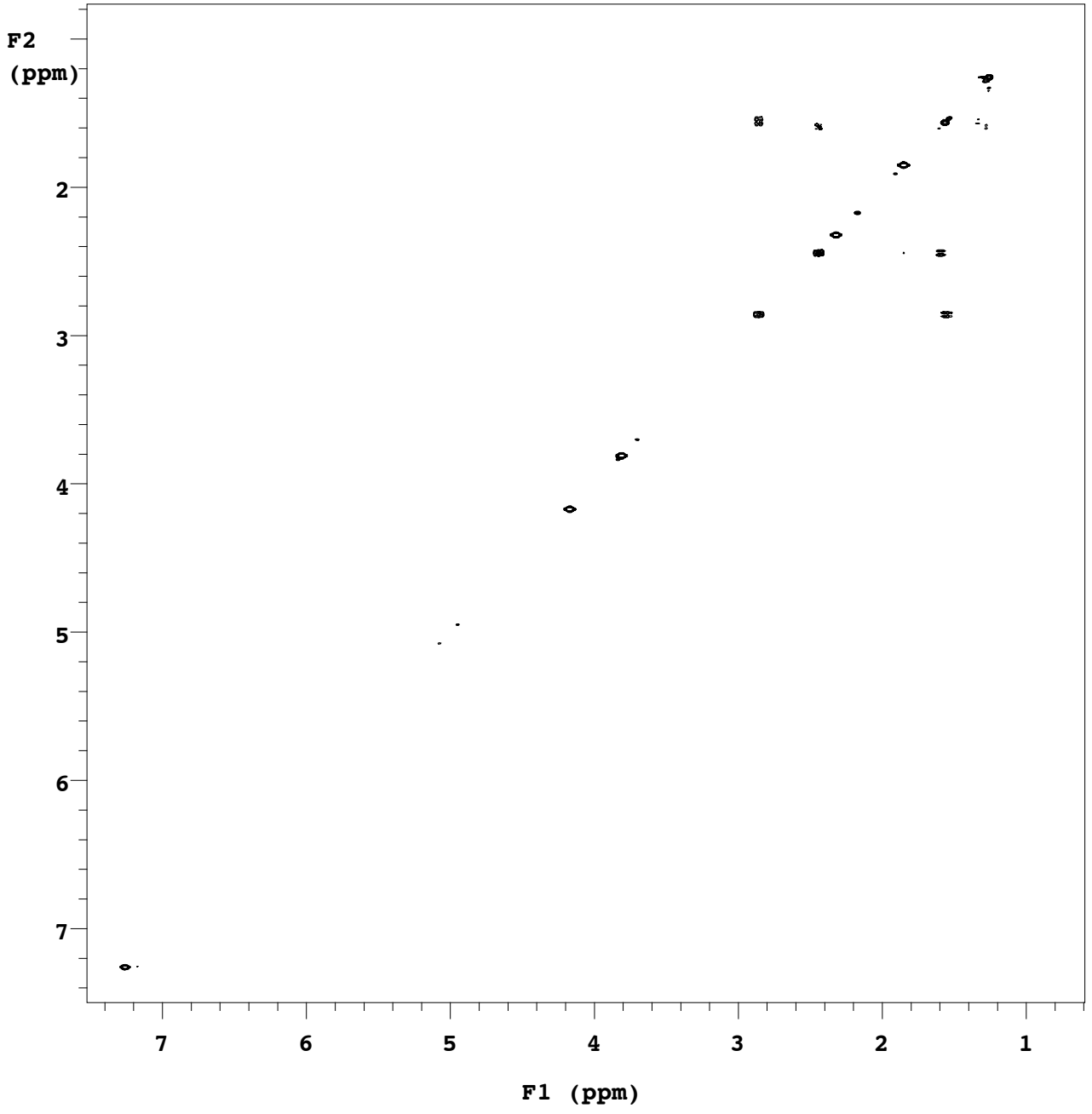


Figure S 24. HSQC spectrum (CDCl3, 1H 600 MHz) of lehualide H (8).

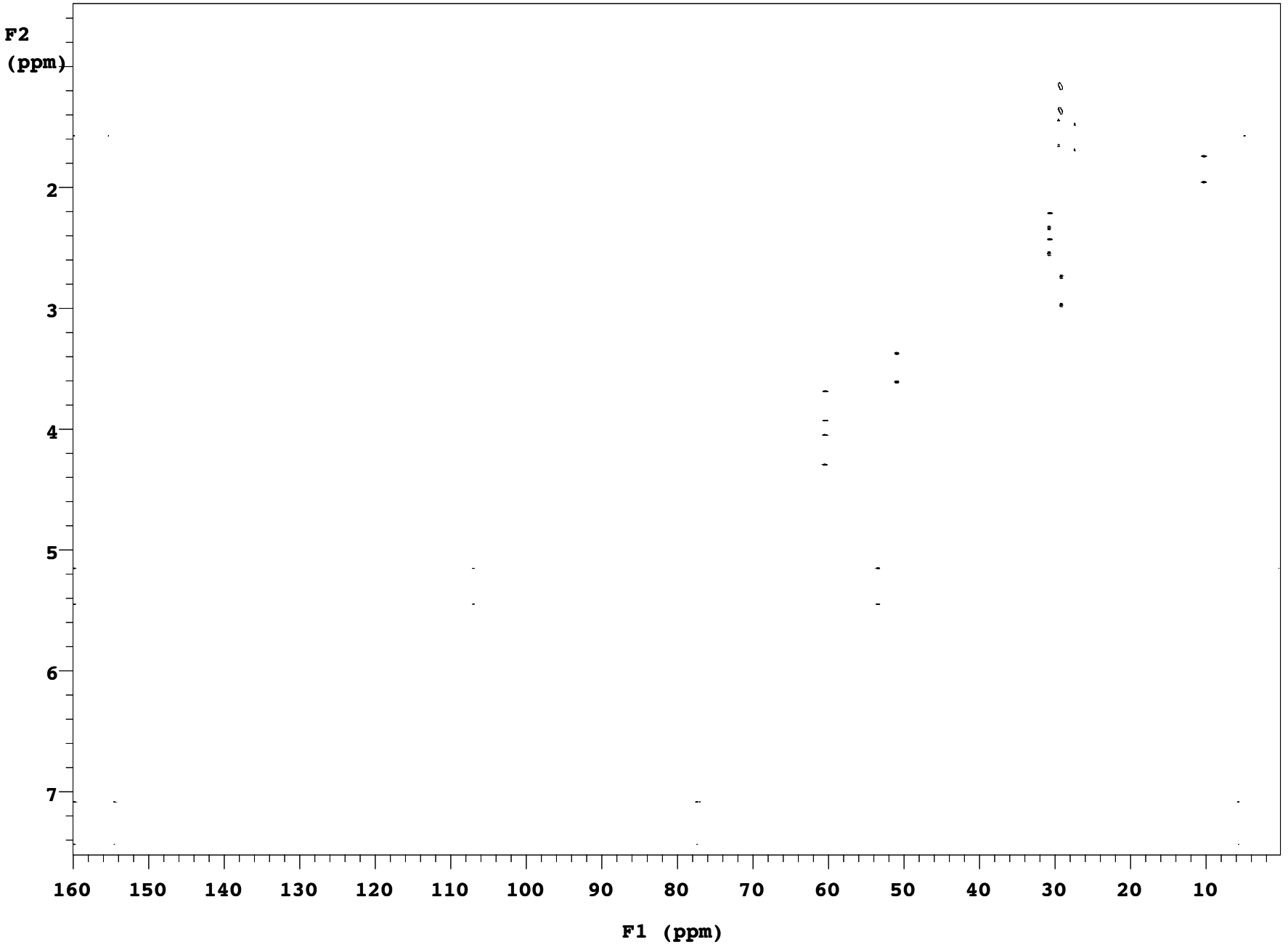


Figure S 25. HMBC spectrum (CDCl3, 1H 600 MHz) of lehualide H (8).

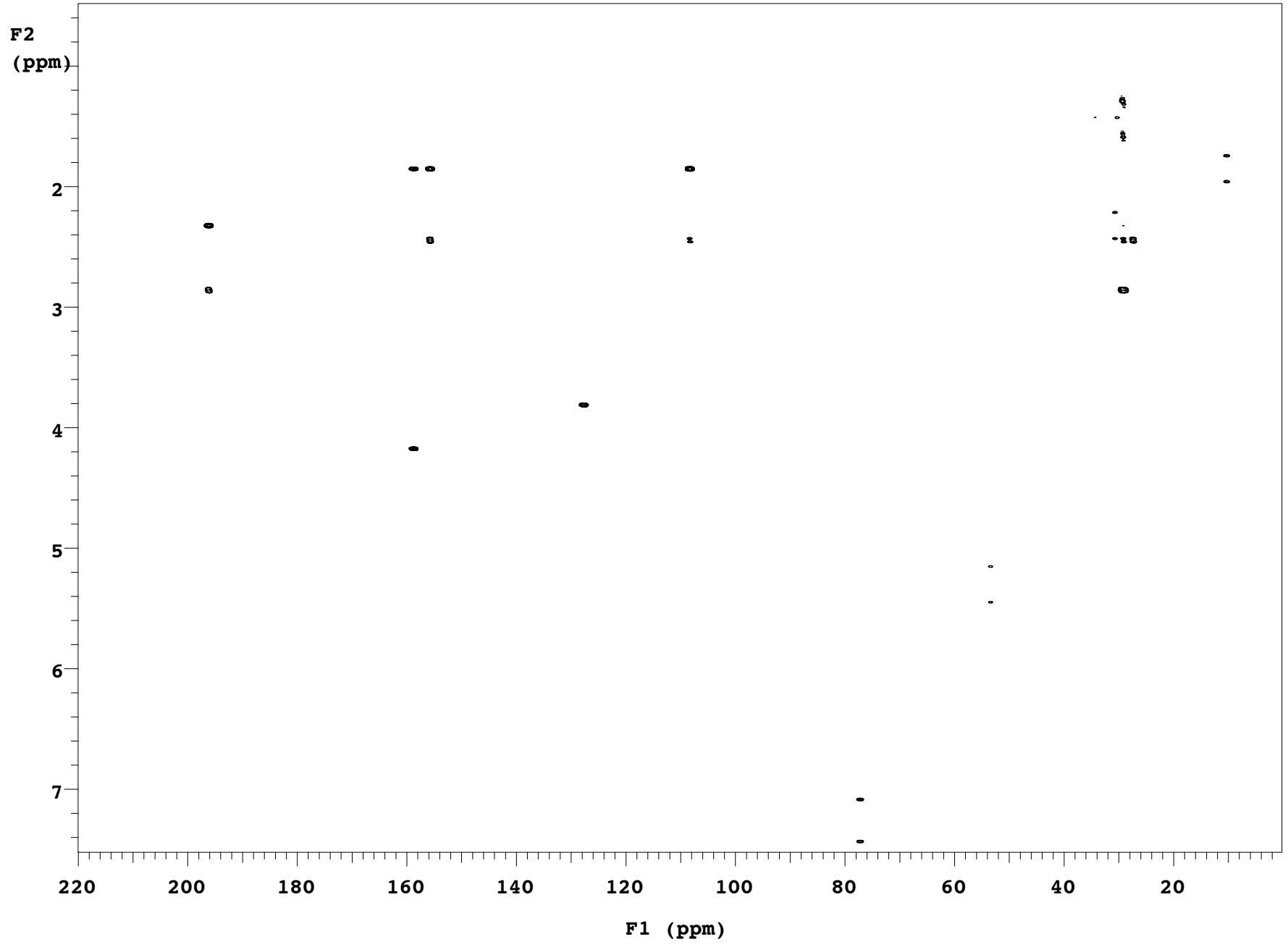
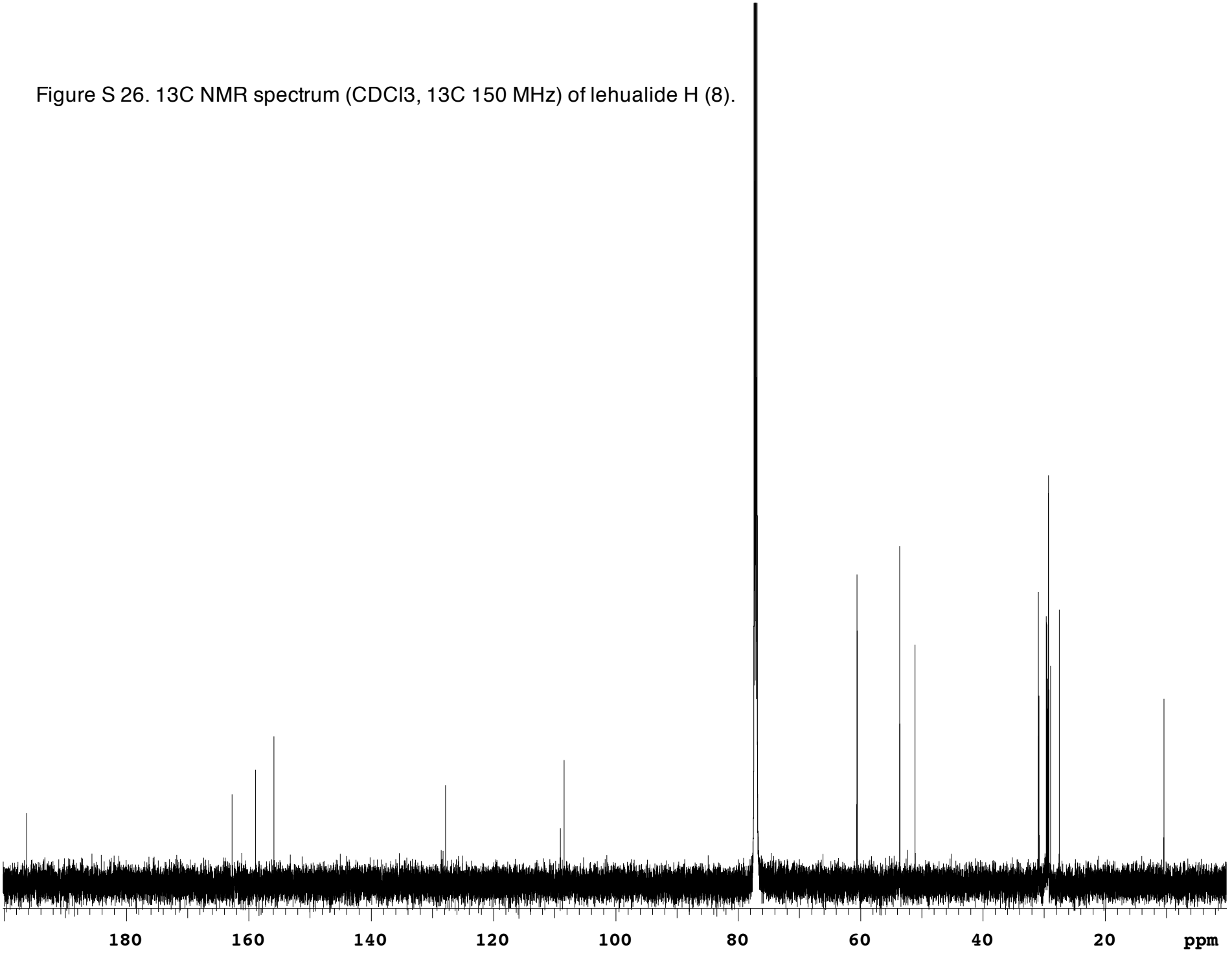


Figure S 26. 13C NMR spectrum (CDCl3, 13C 150 MHz) of lehualide H (8).



Lehualide I (**9**)

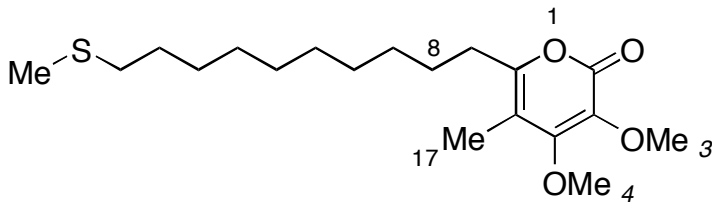


Table S 5. NMR Spectroscopic Data ($CDCl_3$, ^1H 600 MHz; ^{13}C 150 MHz) of Lehualide I (**9**).

			9		
position	**δ_C**	**δ_H**	**COSY**	**HMBC (H → C)**	**NOE[a]**
2	162.6, C				
3	127.7, C				
OCH_3 3	60.4, CH_3	3.85, s		3	*O*CH_3 4
4	158.8, C				
OCH_3 4	60.5, CH_3	4.21, s		4	*O*CH_3 3; 17
5	108.3, C				
6	155.8, C				
7	30.8, CH_2	2.45, t (7.7)	7; 17[b]	8; 6; 5[b]	
8	27.4, CH_2	1.59, quin (7.2)	7; 9	7; 9; 6[b]	
9	29.5, CH_2	1.28, m			
10	29.4, CH_2	1.28, m			
11	29.3, CH_2	1.28, m			
12	29.2, CH_2	1.28, m			
13	29.2, CH_2	1.28, m			
14	28.8, CH_2	1.37, quin (8.0)	15; 13	15; 16; 13	
15	29.2, CH_2	1.58, quin (7.3)	16; 14	16; 14	
16	34.3, CH_2	2.49, bt (7.7)	15; *S*Me[b]	15; *S*Me[b]	
*S*Me	15.6, CH_3	2.09, bs	16[b]	16[b]	
17	10.3, CH_3	1.85, s	7[b]	5; 4; 6	*O*CH_3 4; 7

[a] Selected correlations

[b] Weak correlation

Figure S 27. 1H NMR spectrum (CDCl3, 1H 600 MHz) of lehualide I (9).

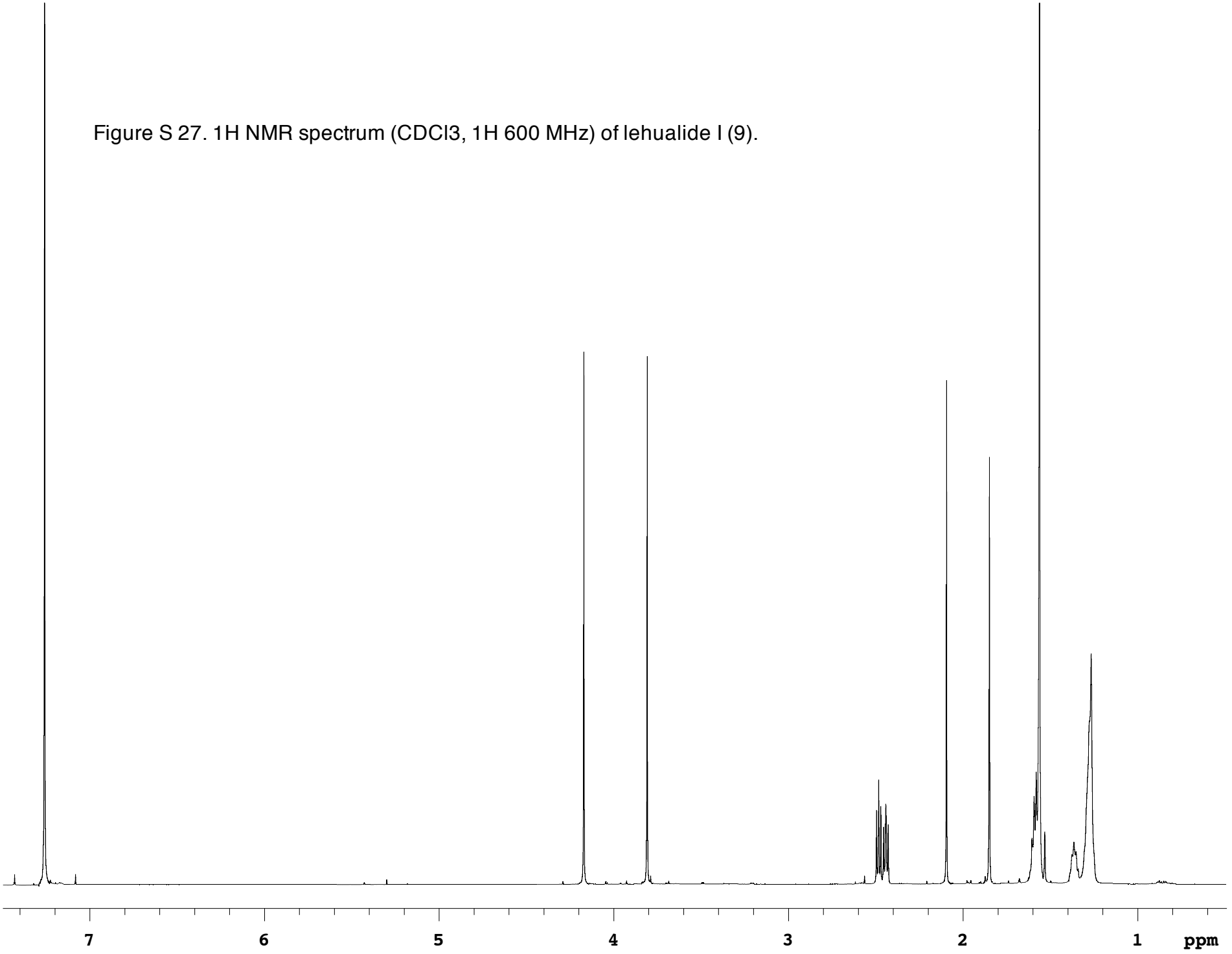


Figure S 28. COSY spectrum (CDCl3, 1H 600 MHz) of lehualide I (9).

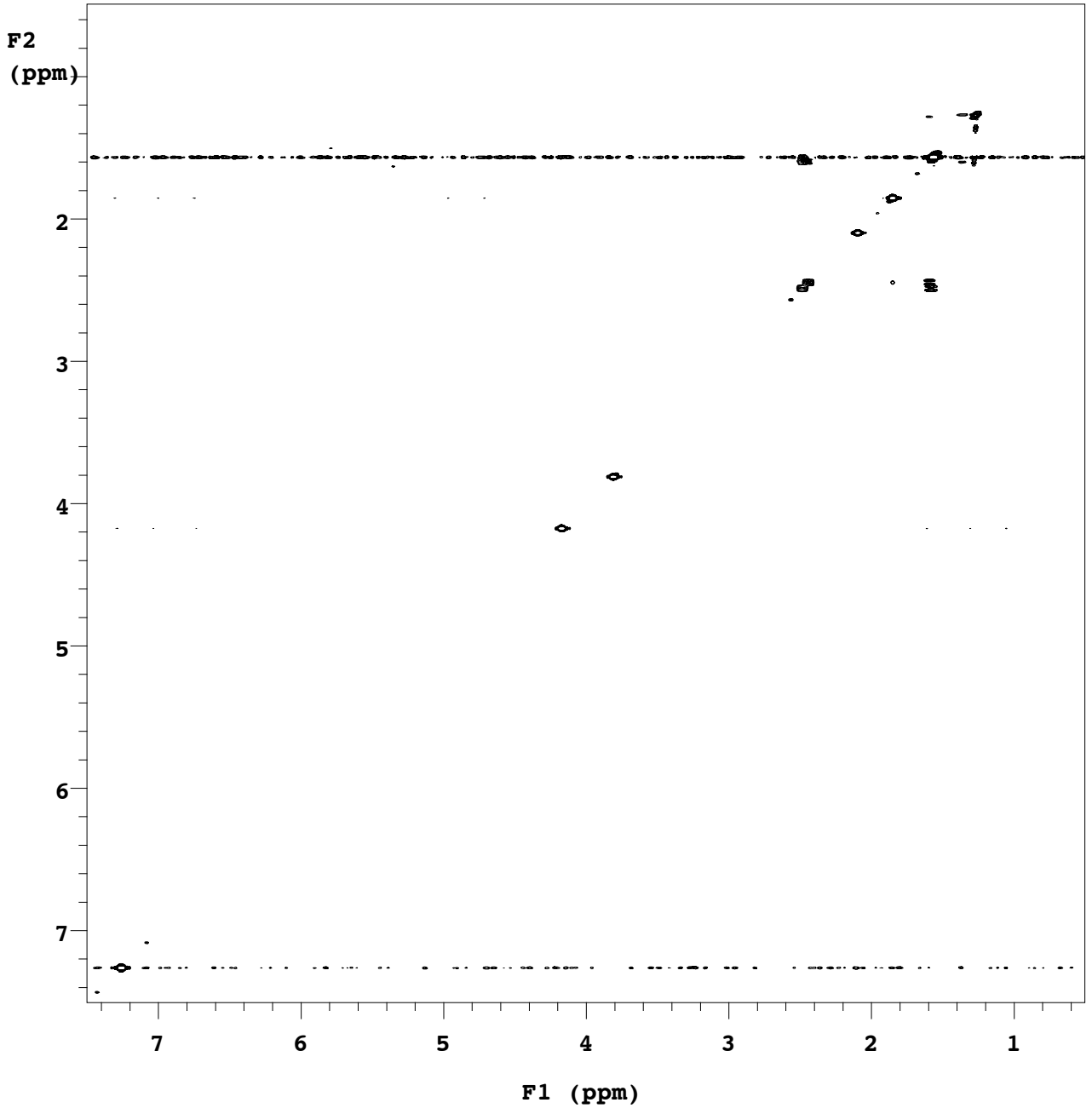


Figure S 29. HSQC spectrum (CDCl3, 1H 600 MHz) of lehualide I (9).

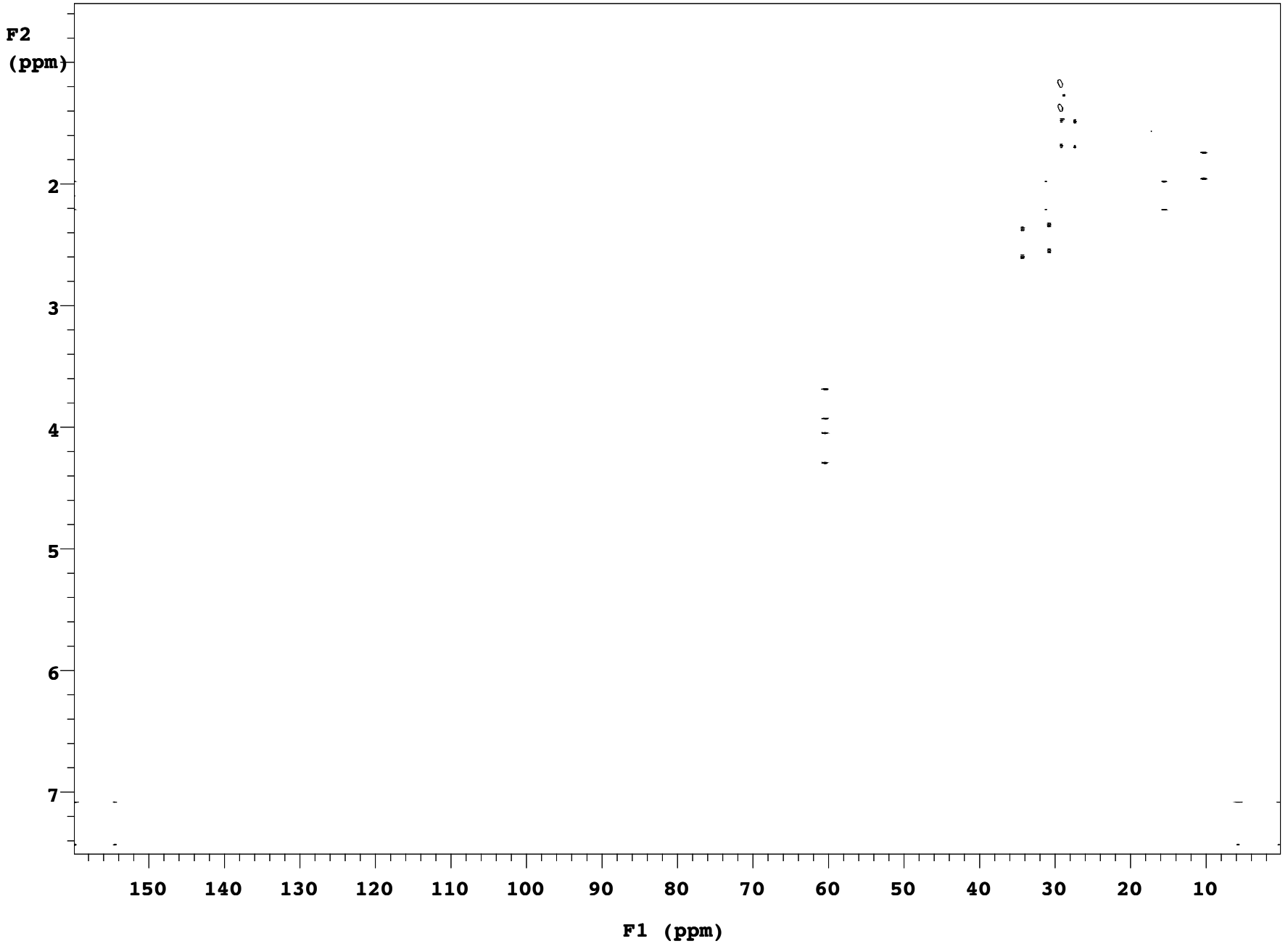


Figure S 30. HMBC spectrum (CDCl3, 1H 600 MHz) of lehualide I (9).

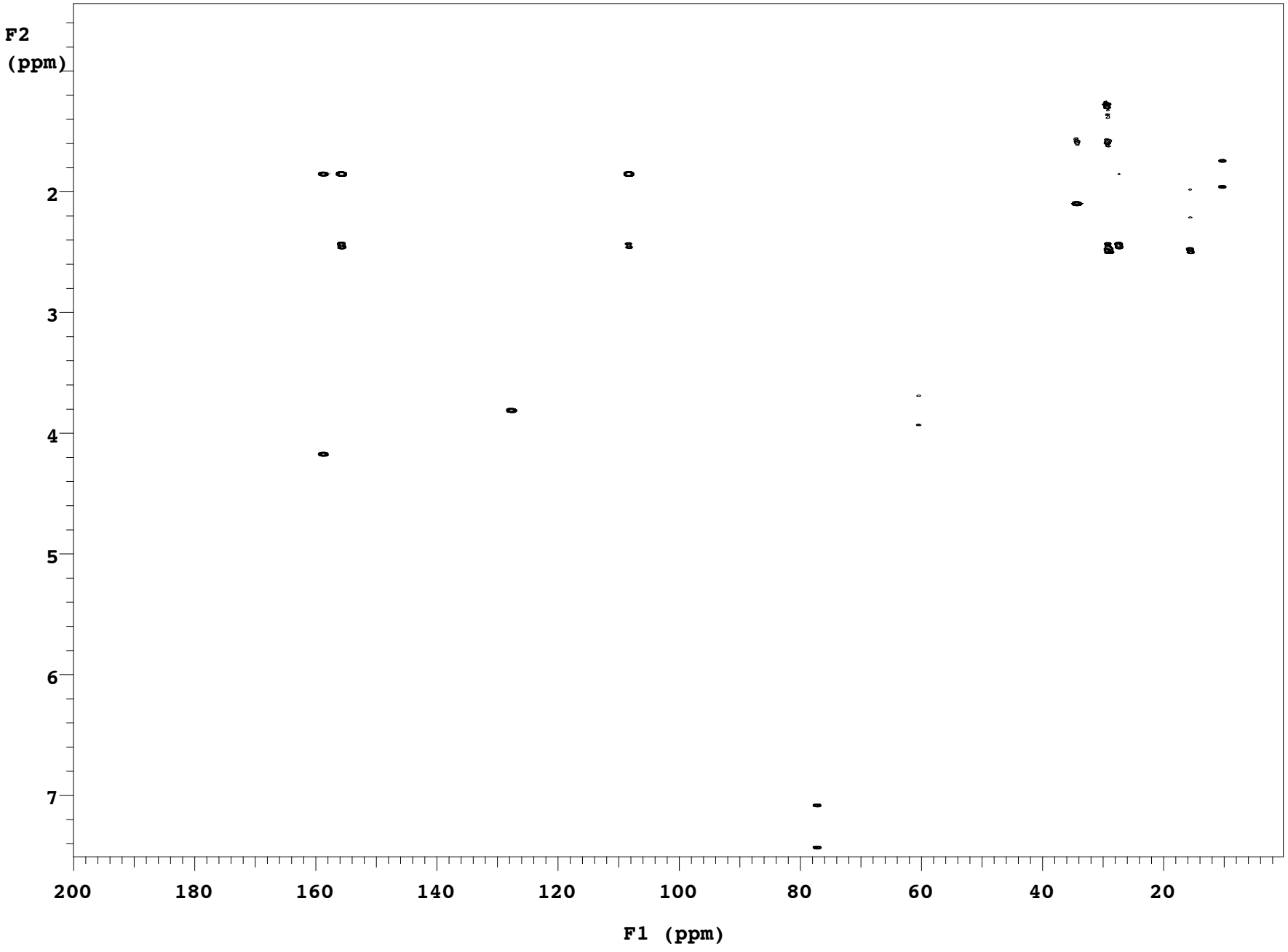
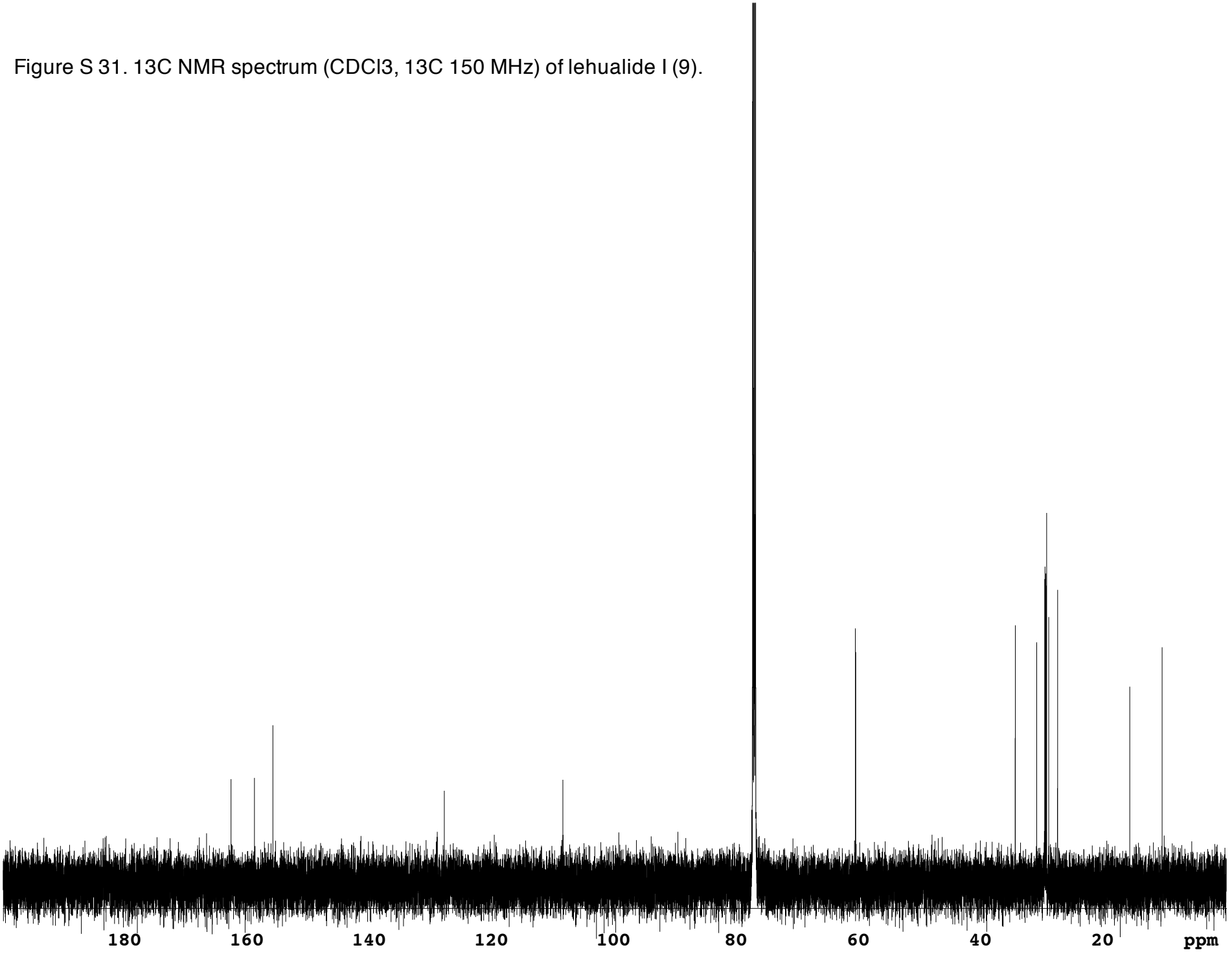


Figure S 31. 13C NMR spectrum (CDCl3, 13C 150 MHz) of lehualide I (9).



Lehualide J (**10**)

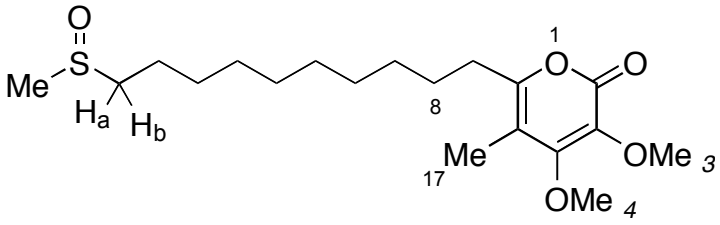


Table S 6. NMR Spectrscopic Data ($CDCl_3$, ^1H 600 MHz; ^{13}C 150 MHz) of Lehualide J (**10**).

		10			
position	**δ_C ,mult**	**δ_H (*J*, Hz)**	**COSY**	**HMBC (H → C)**	**NOE[a]**
2	162.7, C				
3	127.8, C				
OCH_3 3	60.5, CH_3	3.81, s		3	*O*CH_3 4
4	158.9, C				
OCH_3 4	60.6, CH_3	4.17, s		4	*O*CH_3 3; 17
5	108.5, C				
6	155.9, C				
7	30.9, CH_2	2.44, t (7.7)	8; 17[b]	8; 6; 5[b]	17
8	27.5, CH_2	1.59, quin (7.7)	7; 9	7; 9; 6[b]	
9	29.36, CH_2	1.28, m			
10	29.28, CH_2	1.30, m			
11	28.9, CH_2	1.44, m			
12	29.44, CH_2	1.24, m			
13	29.39, CH_2	1.27, m			
14	29.24, CH_2	1.32, m			
15	22.7, CH_2	1.76, quin (7.0)	16a; 16b; 14	14; 16;	
16	54.9, CH_2	a 2.73, ddd (13.0, 9.0, 6.1)	16b; 15	15; 14[b]; O=*S*Me [b]	
		b 2.66, ddd (12.7, 9.2, 6.6)	16a; 15	15; 14[b]; O=*S*Me [b]	
O=*S*Me	38.7, CH_3	2.56, s	16a; 16b	16[b]	
17	10.4, CH_3	1.85, s	7[b]	5; 4; 6	*O*CH_3 4; 7

[a] Selected correlations

[b] Weak correlation

Figure S 32. 1H NMR spectrum (CDCl3, 1H 600 MHz) of lehualide J (10).

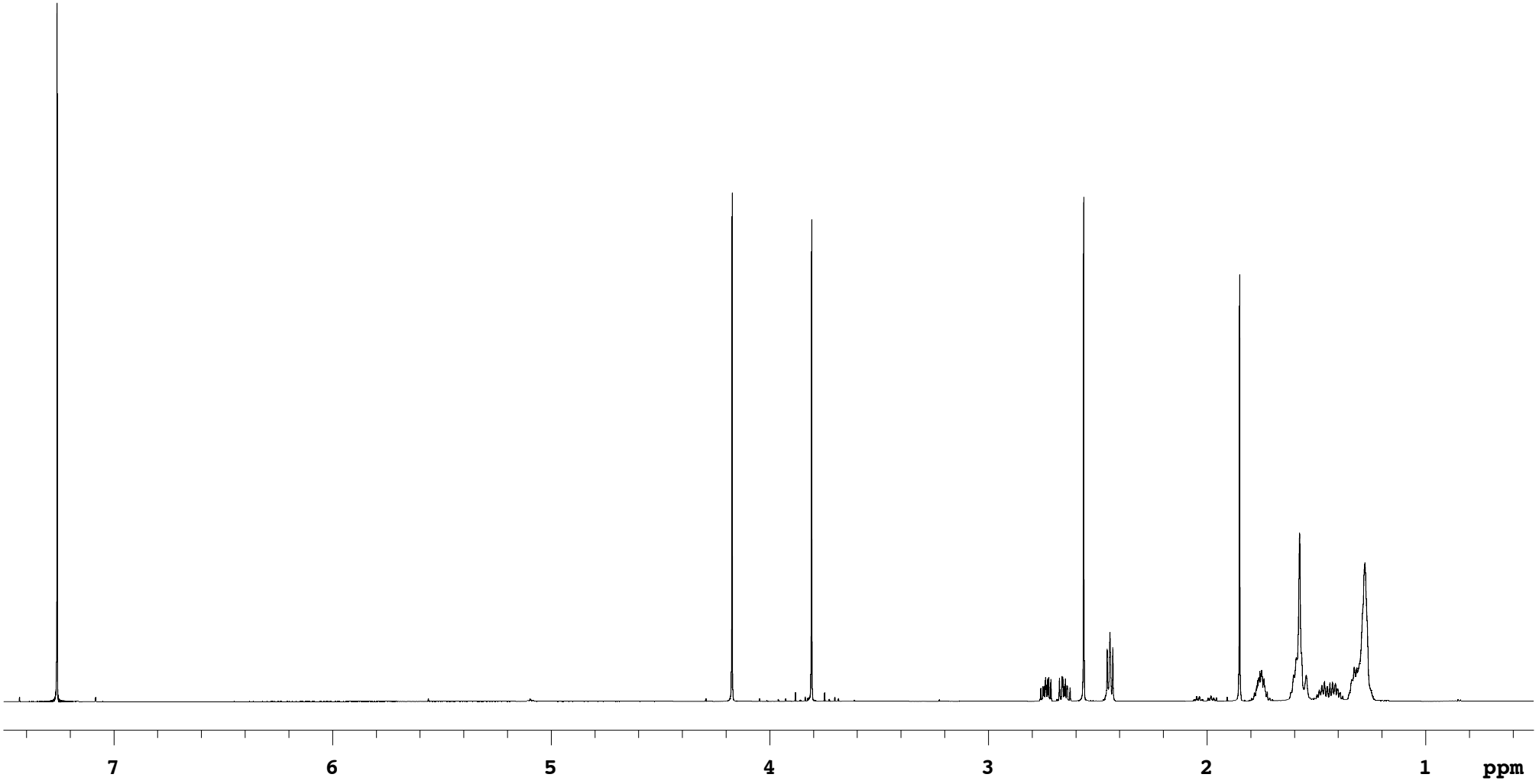


Figure S 33. COSY spectrum (CDCl3, 1H 600 MHz) of lehualide J (10).

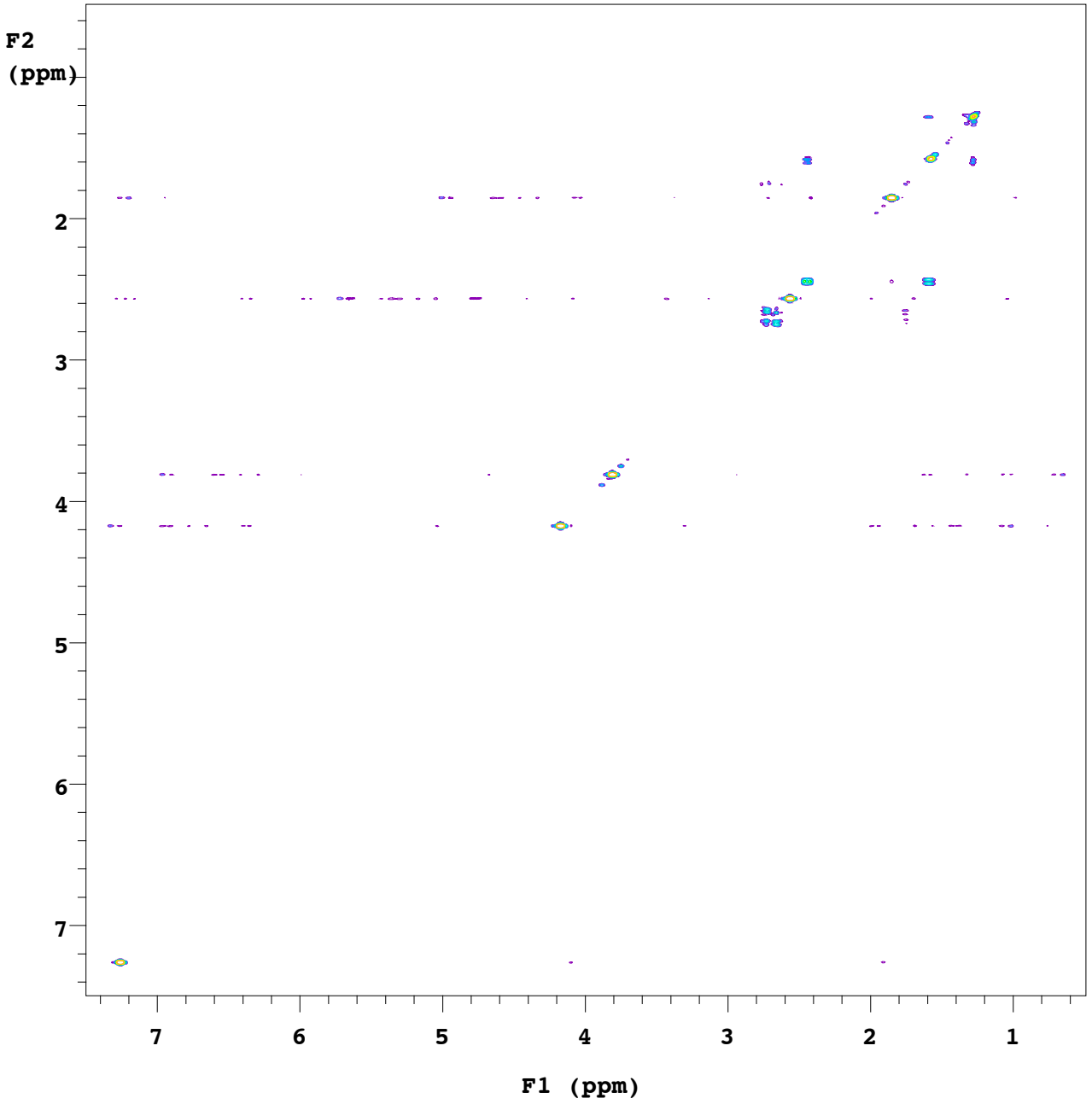


Figure S 34. HSQC spectrum (CDCl3, 1H 600 MHz) of lehualide J (10).

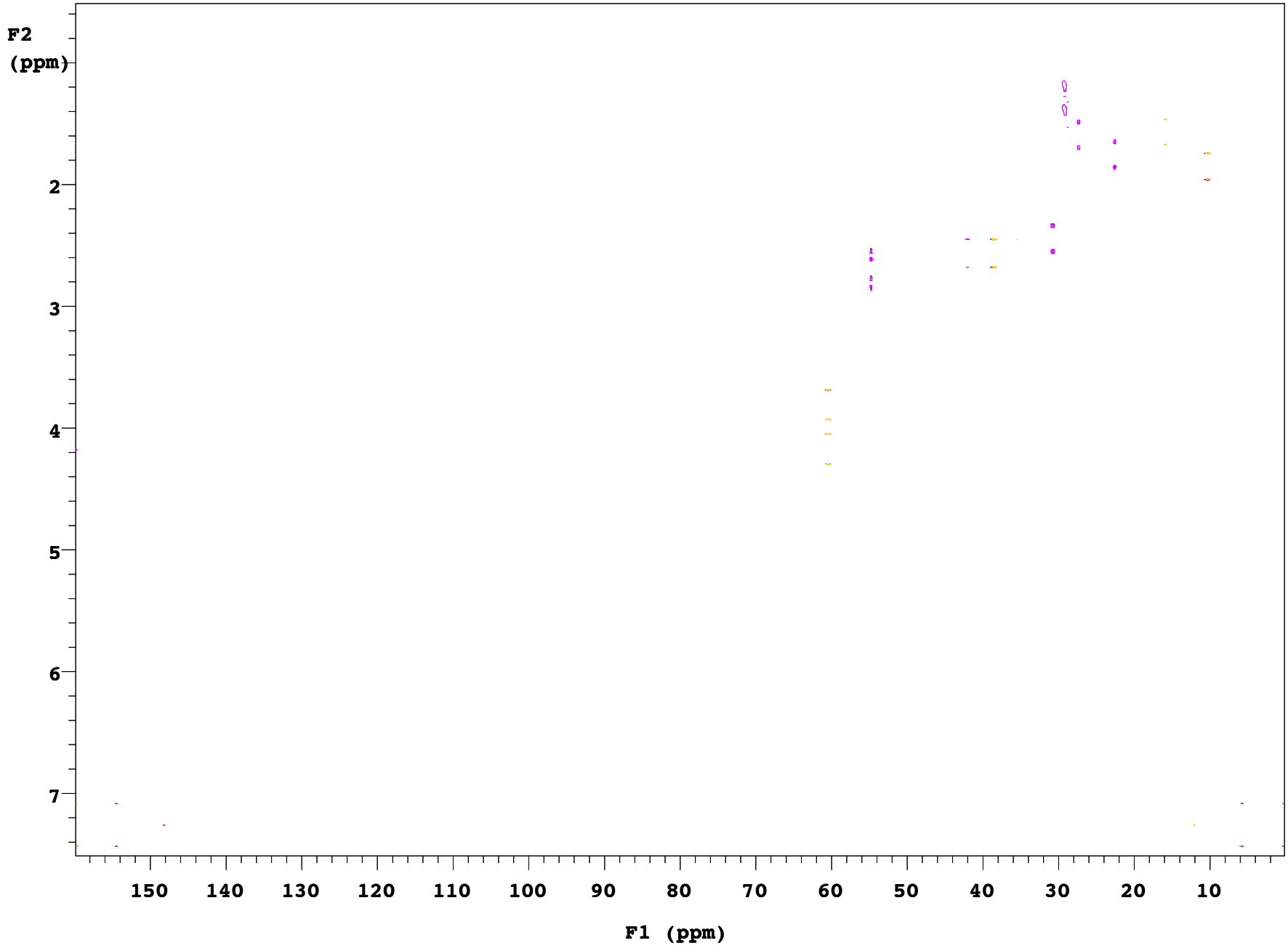


Figure S 35. HMBC spectrum (CDCl3, 1H 600 MHz) of lehualide J (10).

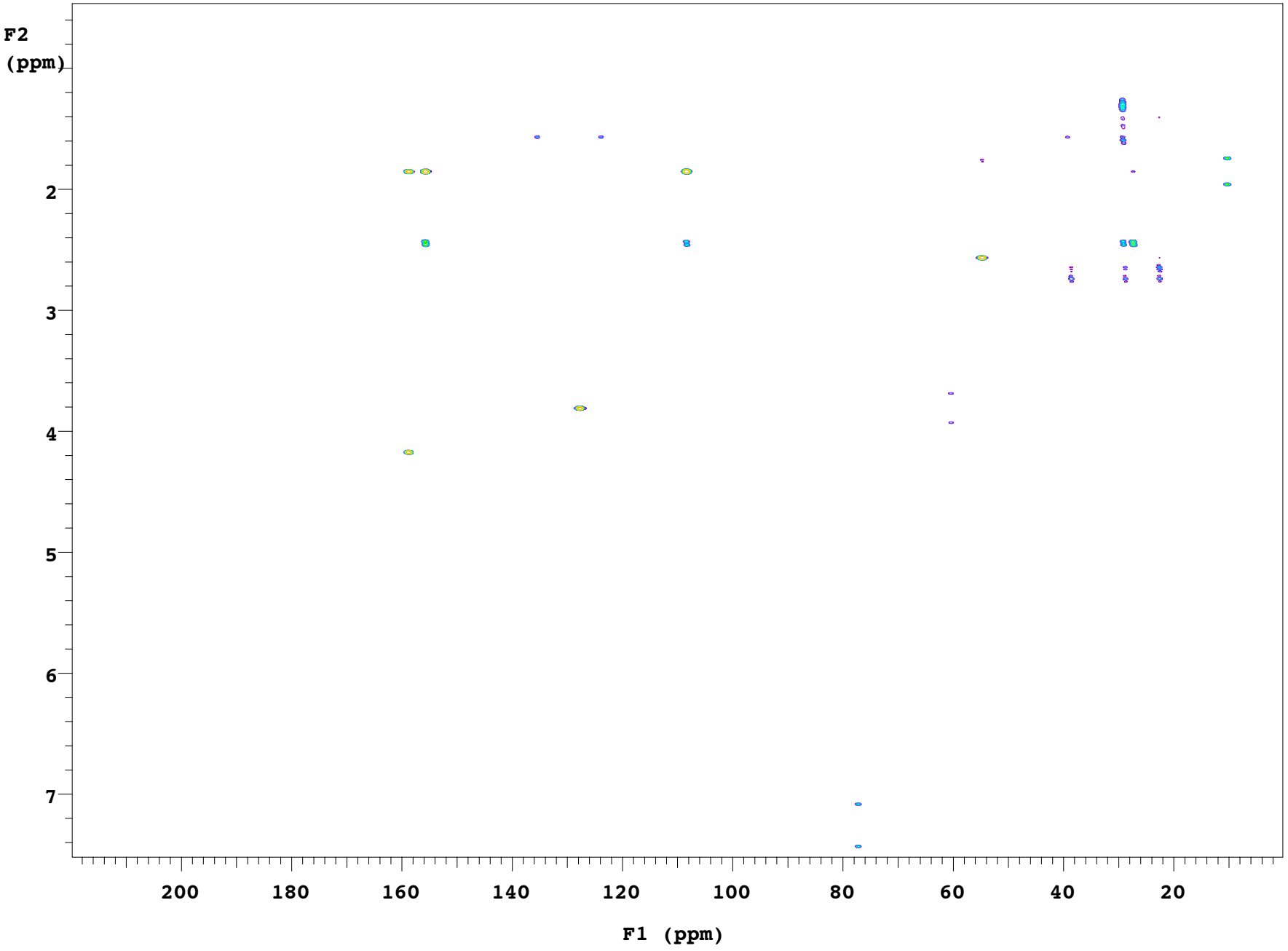
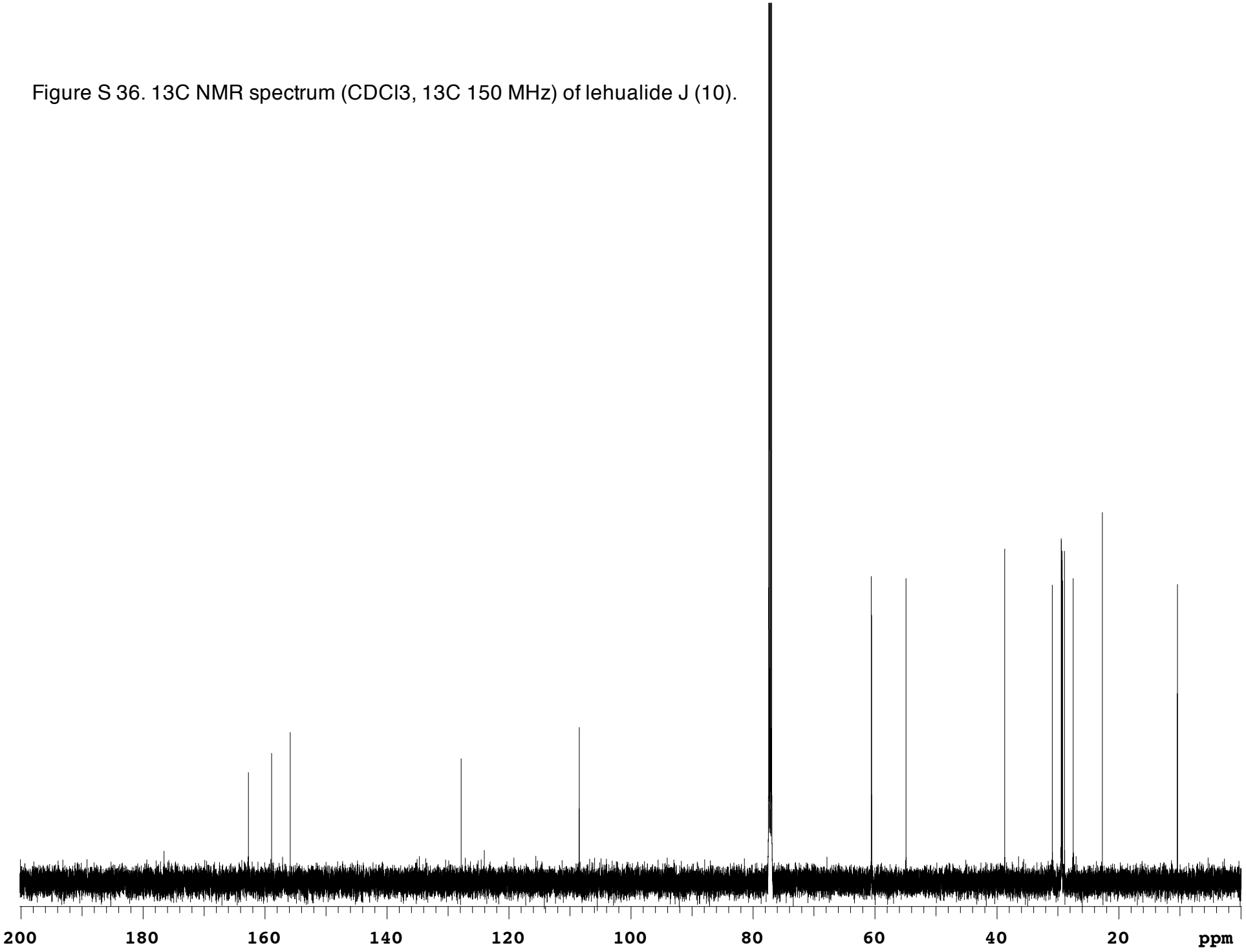


Figure S 36. 13C NMR spectrum (CDCl3, 13C 150 MHz) of lehualide J (10).



Lehualide K (**11**)

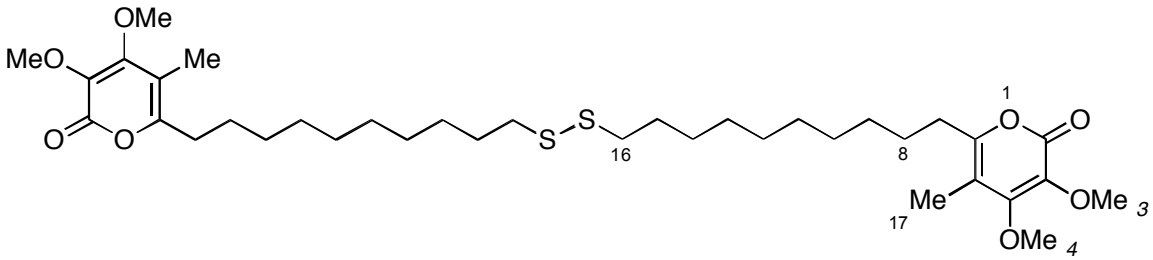


Table S 7. NMR Spectroscopic Data ($CDCl_3$, ^1H 600 MHz; ^{13}C 150 MHz) of Lehualide K (**11**).

		11			
position	**δ_C , mult**	**δ_H (*J*, Hz)**	**COSY**	**HMBC (H → C)**	**NOE[a]**
2	162.7, C				
3	128.4, C				
OCH_3 3	60.5, CH_3	3.81, s		3	*O*CH_3 4
4	158.9, C				
OCH_3 4	60.6, CH_3	4.17, s		4	*O*CH_3 3; 17
5	108.5, C				
6	155.9, C				
7	30.9, CH_2	2.44, t (7.7)	8; 17[b]	8; 6; 9; 5[b]	17
8	27.5, CH_2	1.59, quin (7.5)	7; 9	7; 9; 6[b]	
9	29.33, CH_2	1.27, m			
10	29.62, CH_2	1.28, m			
11	29.59, CH_2	1.28, m			
12	29.55, CH_2	1.28, m			
13	29.44, CH_2	1.28, m			
14	28.6, CH_2	1.37, quin (7.6)	13; 15	15; 16; 13	
15	29.3, CH_2	1.66, quin (7.4)	14; 16	14; 16; 15	
16	39.2, CH_2	2.67, t (7.4)			
17	10.4, CH_3	1.84, s	7[b]	4; 5; 6	*O*CH_3 4; 7

[a] Selected correlations

[b] Weak correlation

Figure S 37. 1H NMR spectrum (CDCl3, 1H 600 MHz) of lehualide K (11).

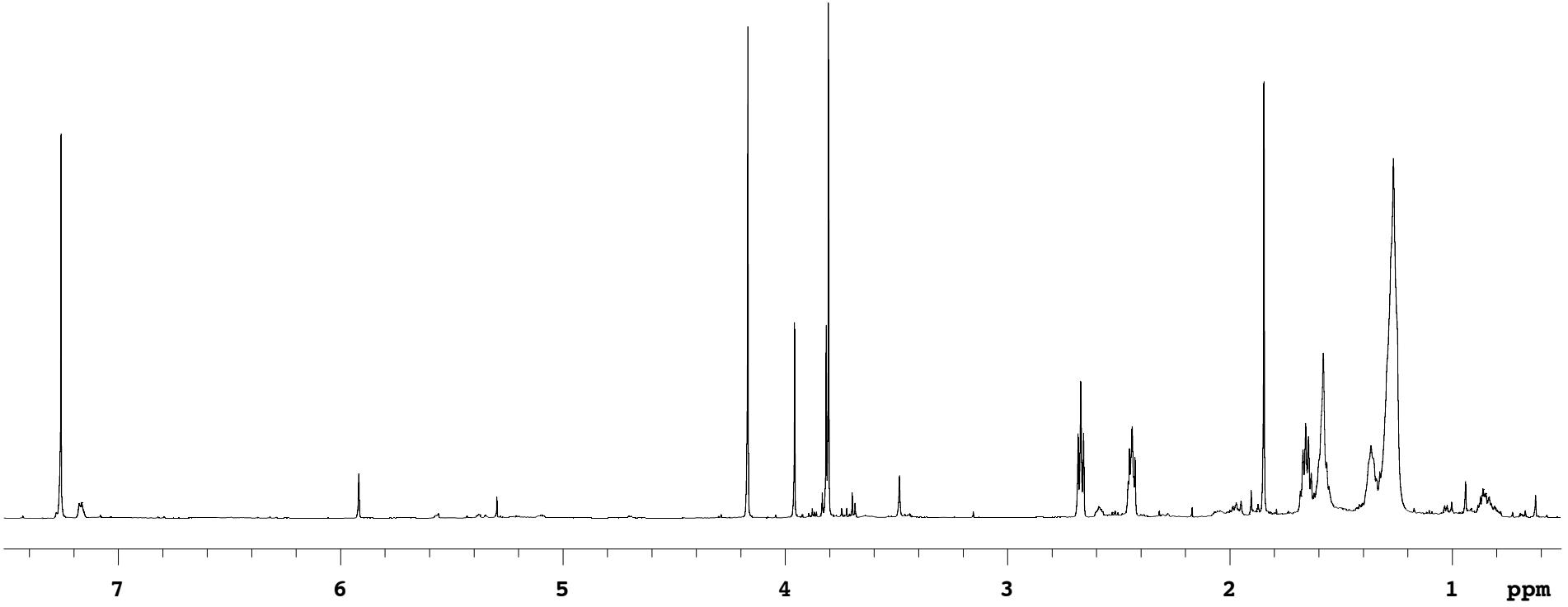


Figure S 38. COSY spectrum (CDCl3, 1H 600 MHz) of lehualide K (11).

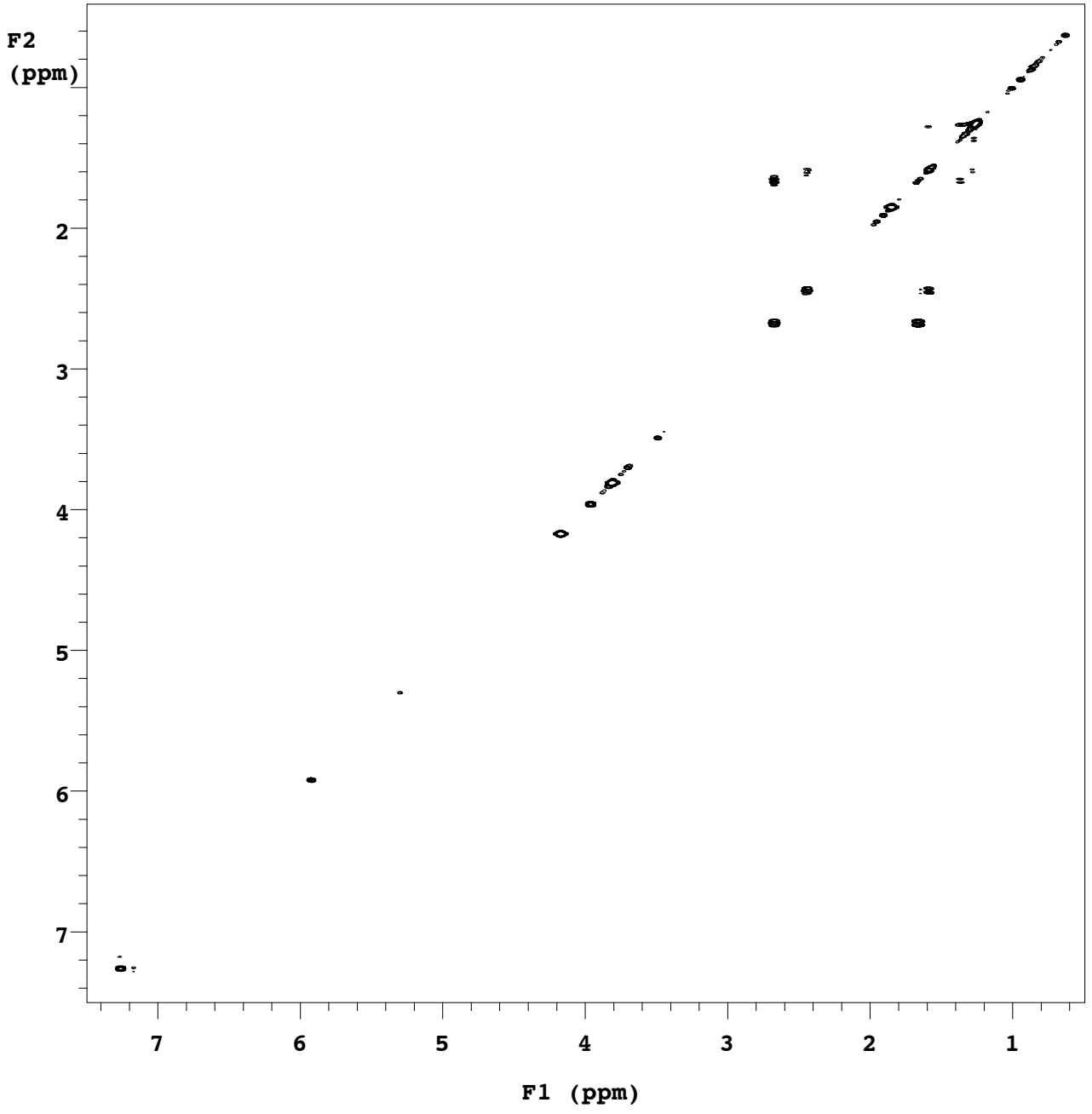


Figure S 39. HSQC spectrum (CDCl3, 1H 600 MHz) of lehualide K (11).

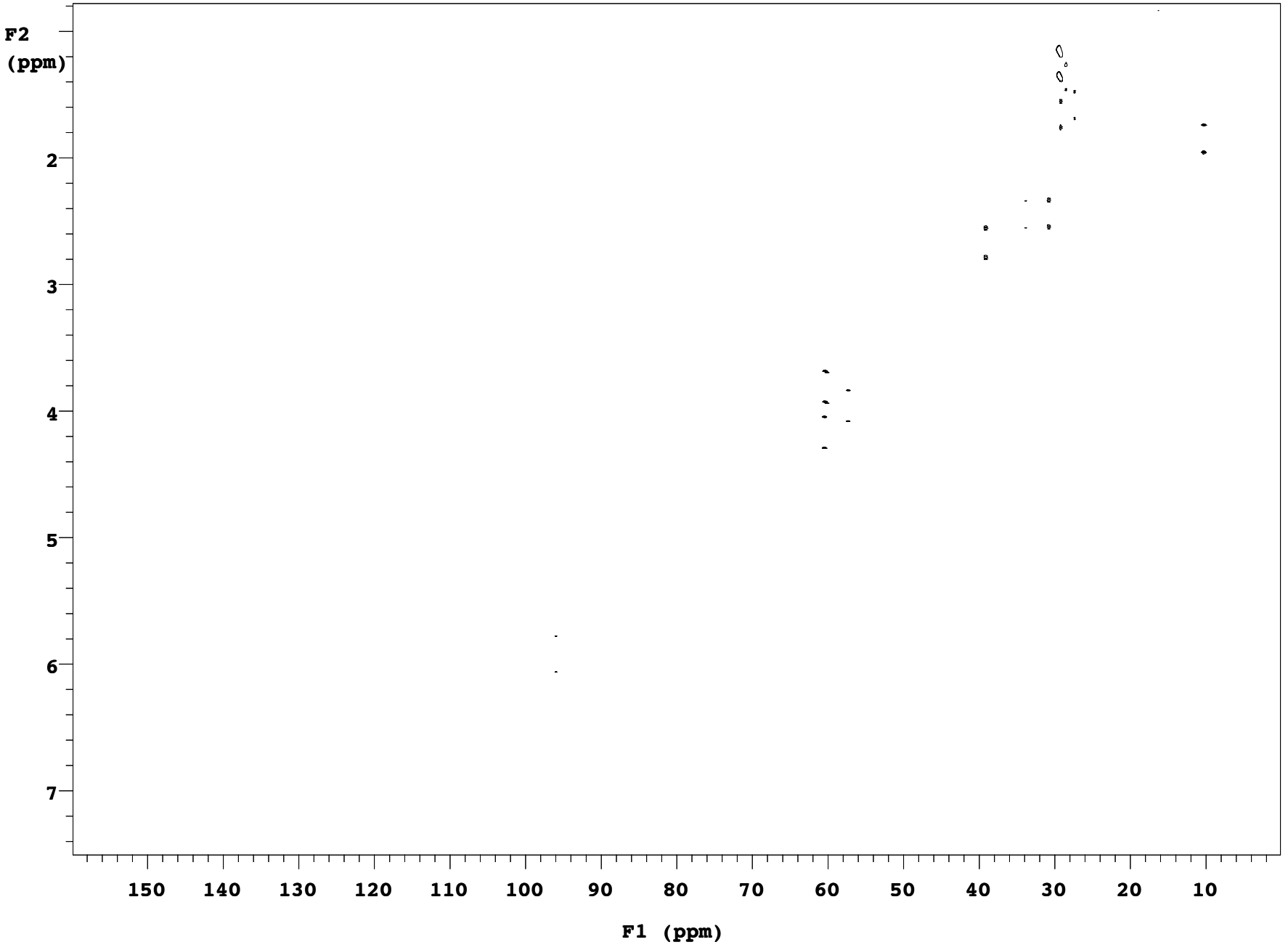


Figure S 40. HMBC spectrum (CDCl3, 1H 600 MHz) of lehualide K (11).

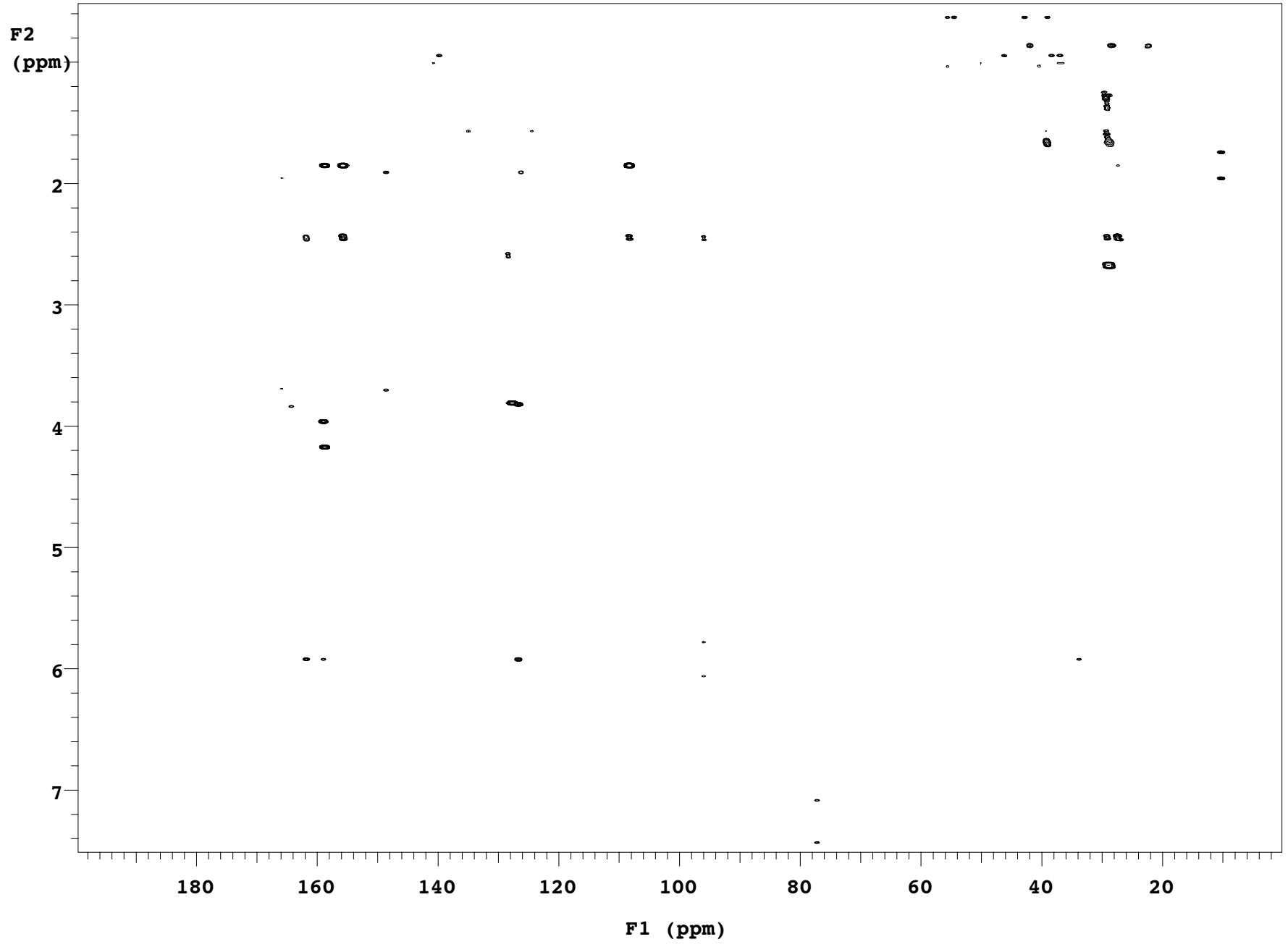
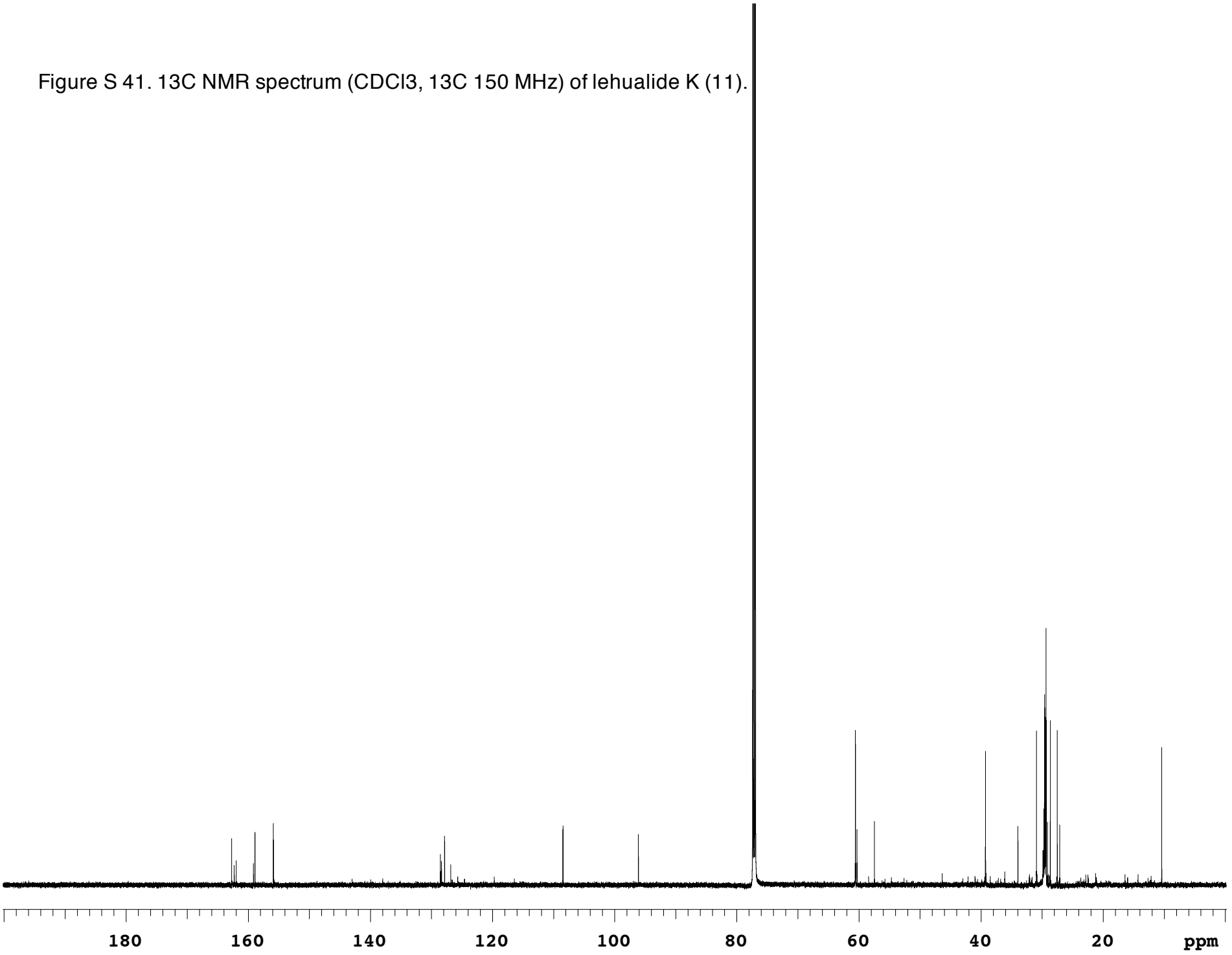


Figure S 41. 13C NMR spectrum (CDCl3, 13C 150 MHz) of lehualide K (11).



Plakortis species

Figure S 42. Above-water photograph of *Plakortis* sp. analyzed.